Introduction to Unsupervised Learning

Legal Notices and Disclaimers

Types of Machine Learning

Supervised	data points have known outcome
Unsupervised	data points have unknown outcome

Types of Machine Learning

Supervised — data points have known outcome

Unsupervised — data points have unknown outcome

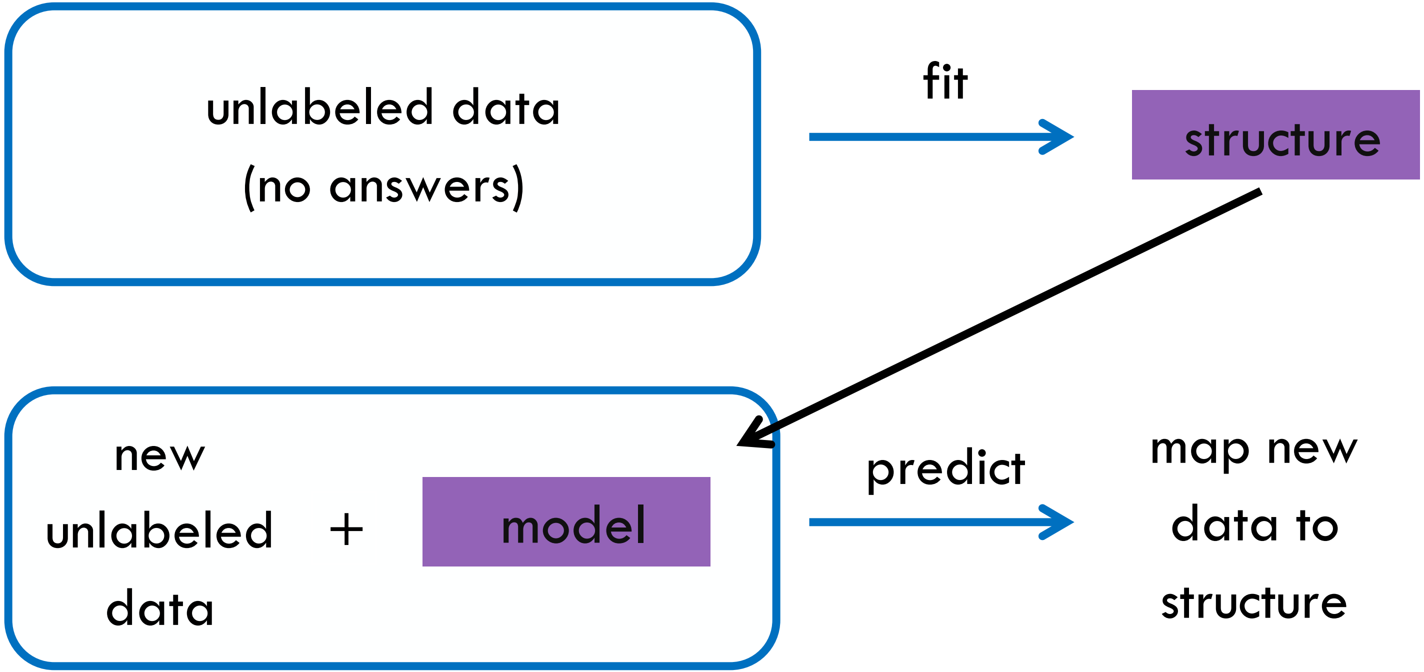
Types of Unsupervised Learning

Clustering identify unknown structure in data

Types of Unsupervised Learning

Clustering	identify unknown structure in data
Dimensionality Reduction	use structural characteristics to simplify data

Unsupervised Learning Overview

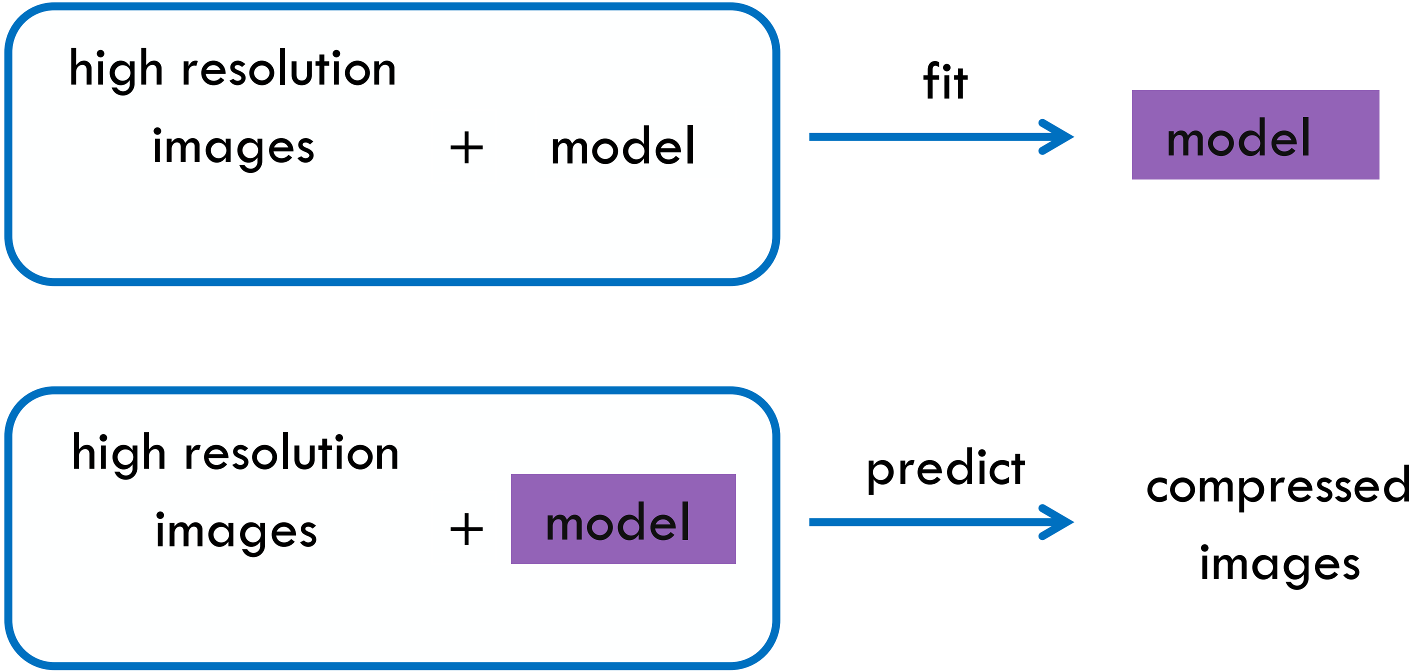


Clustering: Finding Distinct Groups

text articles of unknown topics + model $\xrightarrow{\text{fit}}$ model

text articles of unknown topics + model $\xrightarrow{\text{predict}}$ predict similar articles

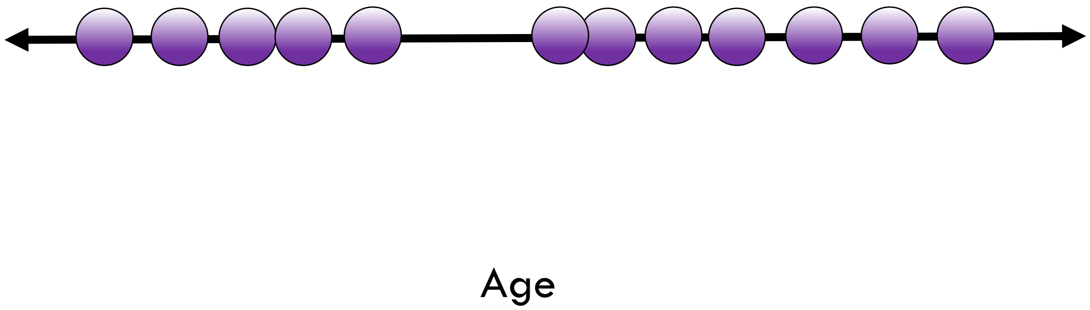
Dimensionality Reduction: Simplifying Structure



Introduction to Unsupervised Learning

Users of a web application:

One feature (age)



Introduction to Unsupervised Learning

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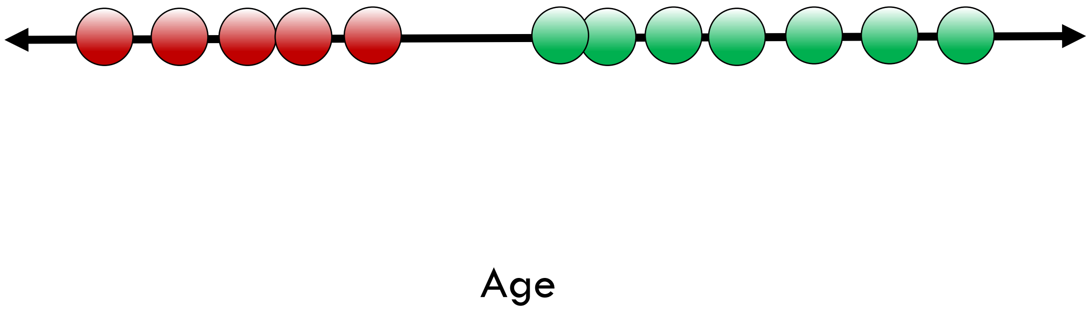
One feature (age)

Two clusters

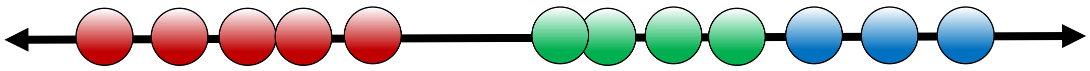


Introduction to Unsupervised Learning

Users of a web application:

One feature (age)

Three clusters



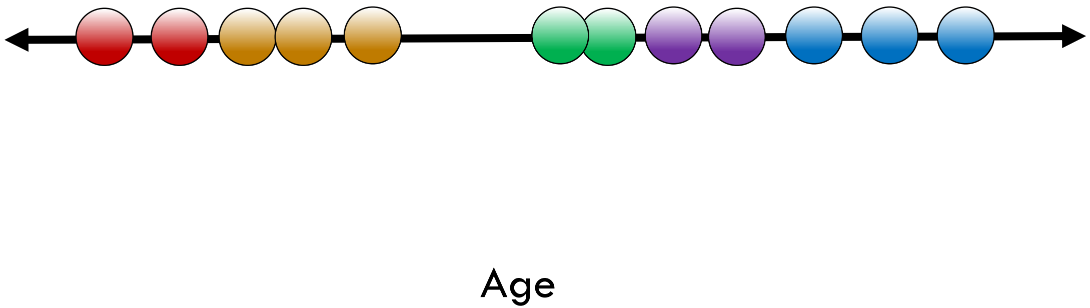
Age

Introduction to Unsupervised Learning

Users of a web application:

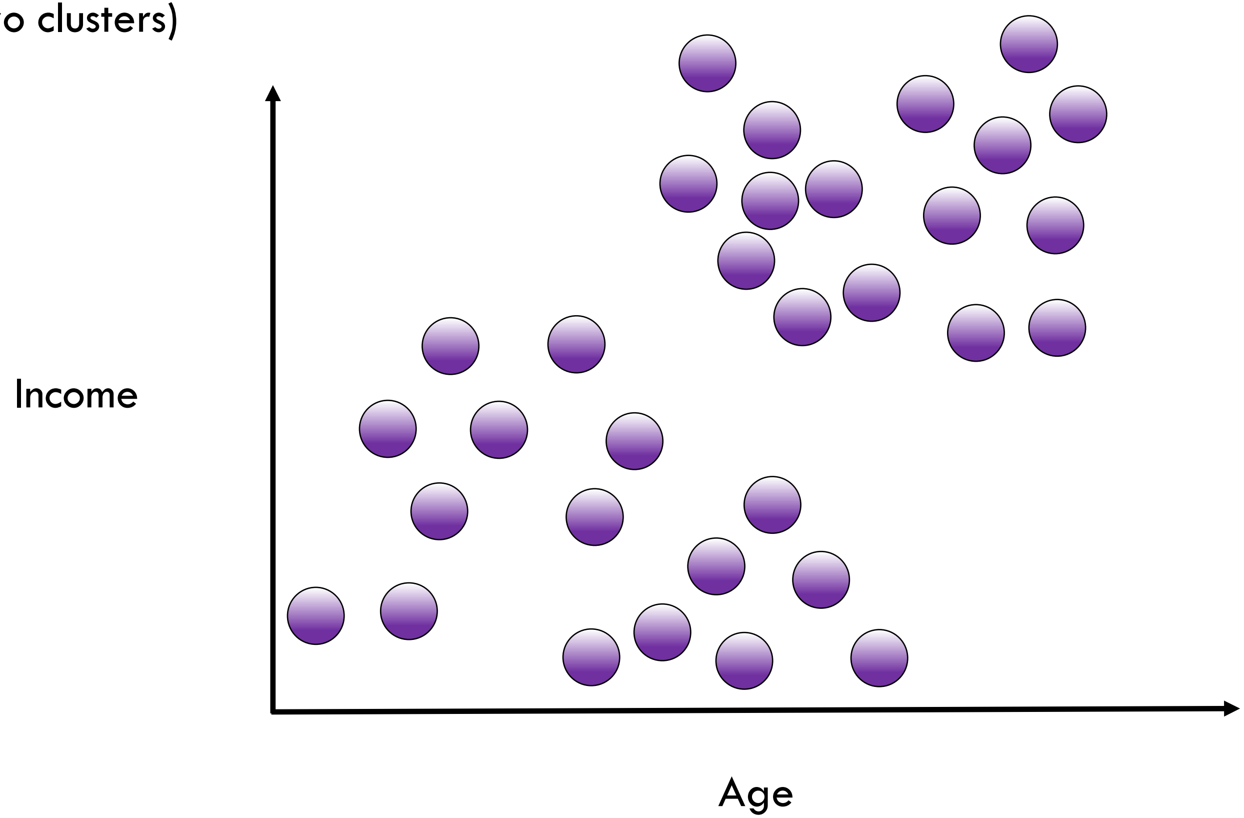
One feature (age)

Five clusters



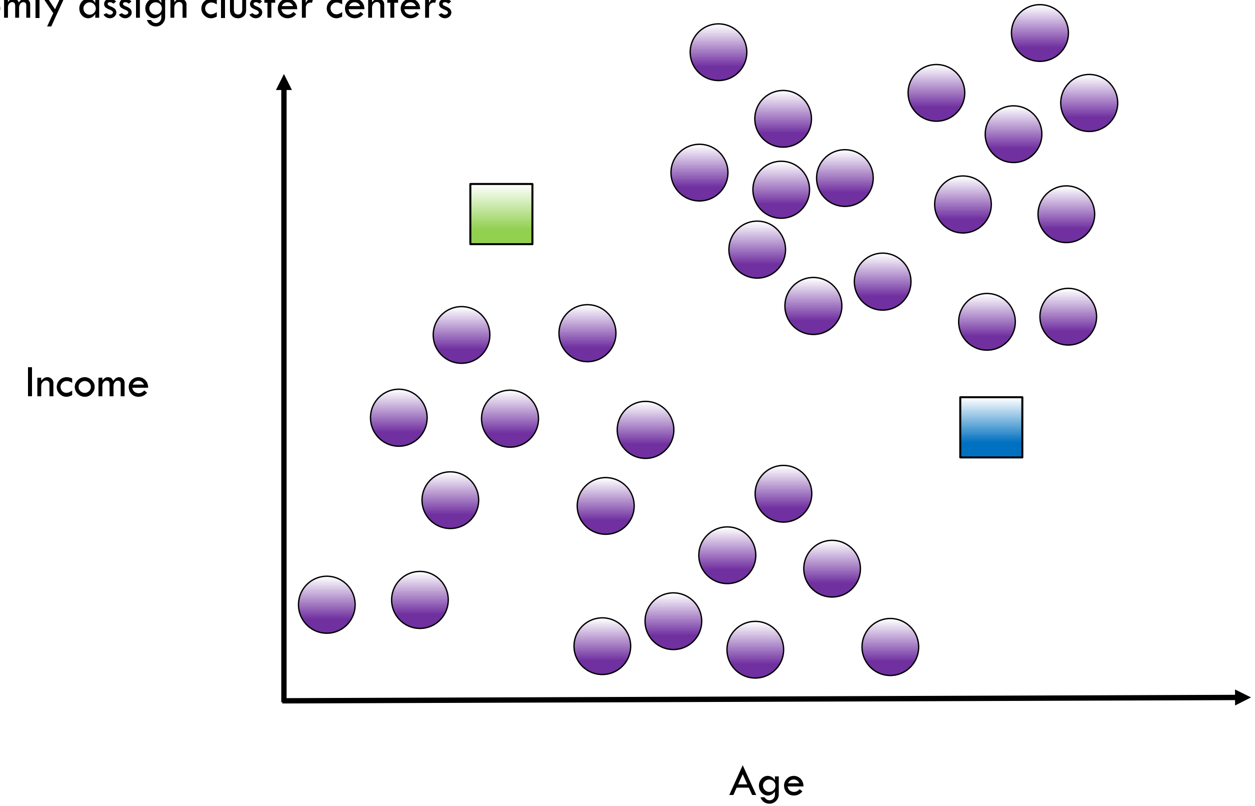
K-Means Algorithm

K = 2 (find two clusters)



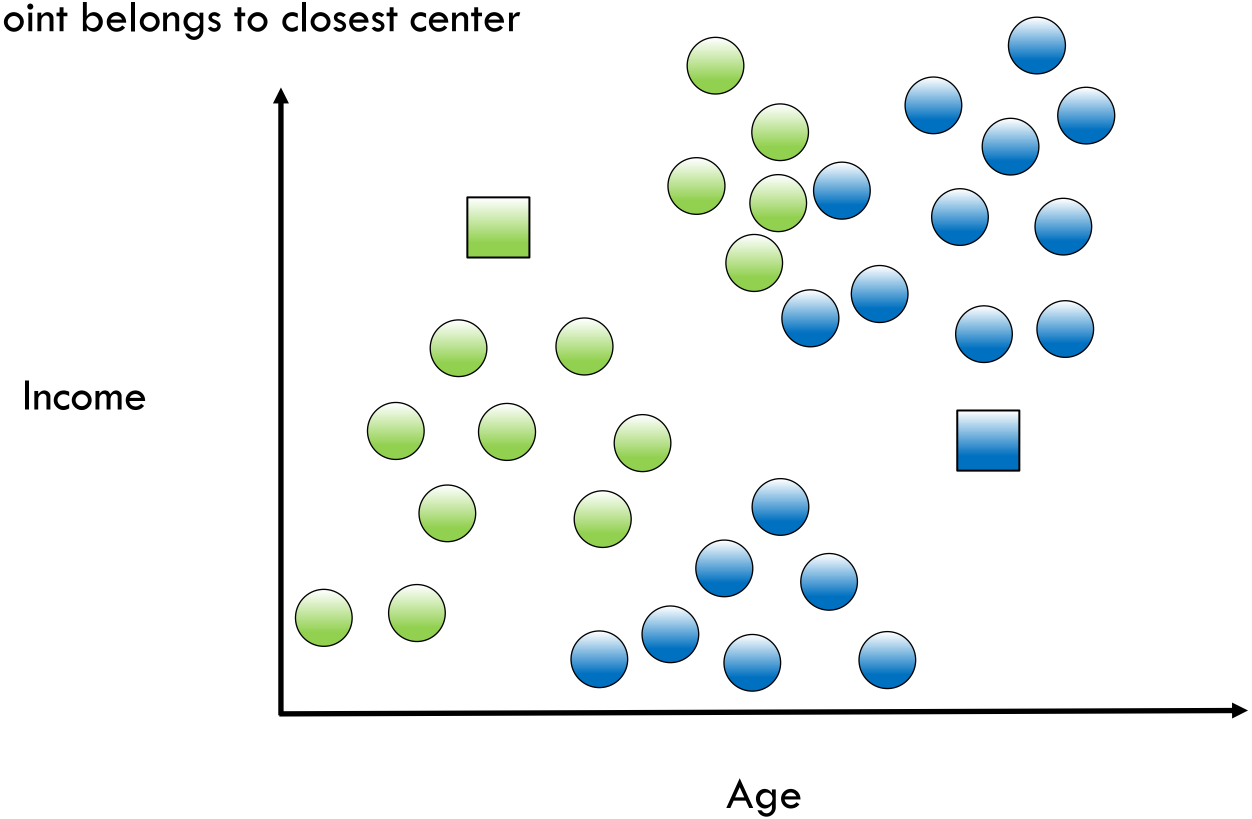
K-Means Algorithm

K = 2, Randomly assign cluster centers



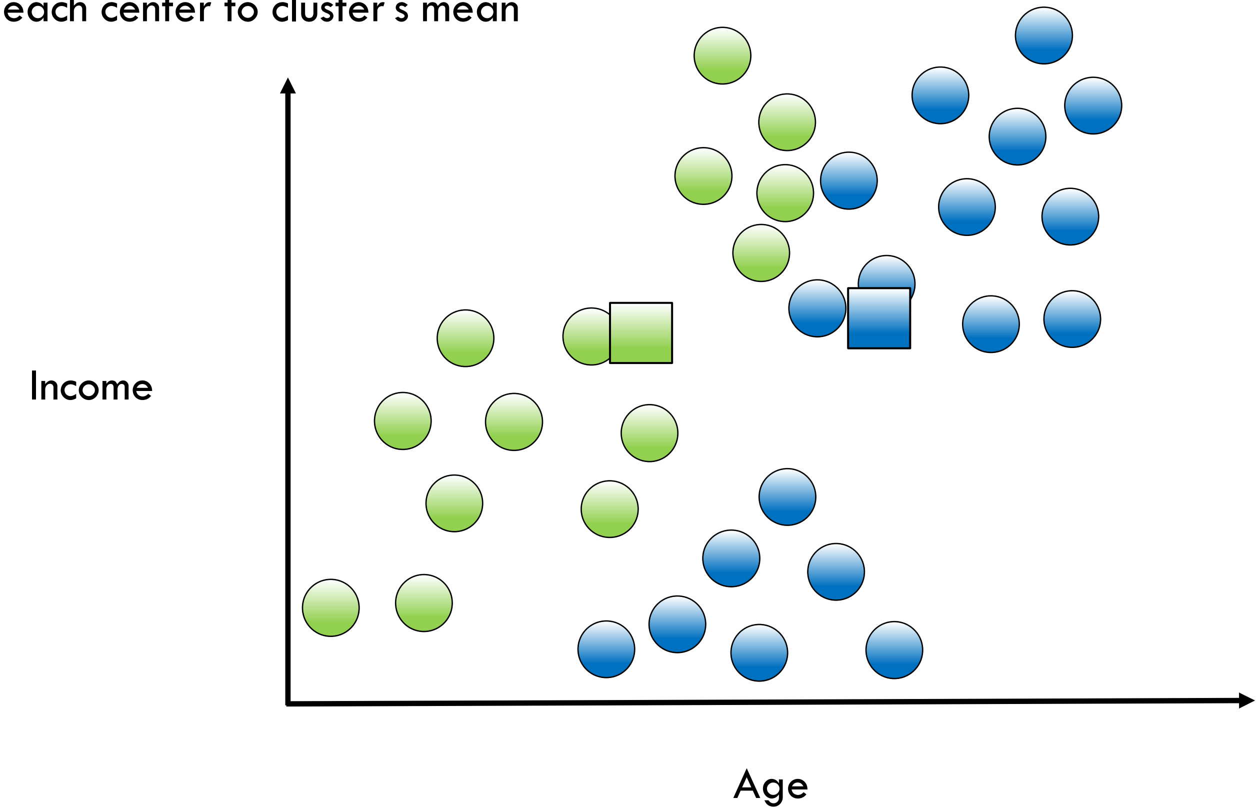
K-Means Algorithm

K = 2, Each point belongs to closest center



K-Means Algorithm

K = 2, Move each center to cluster's mean



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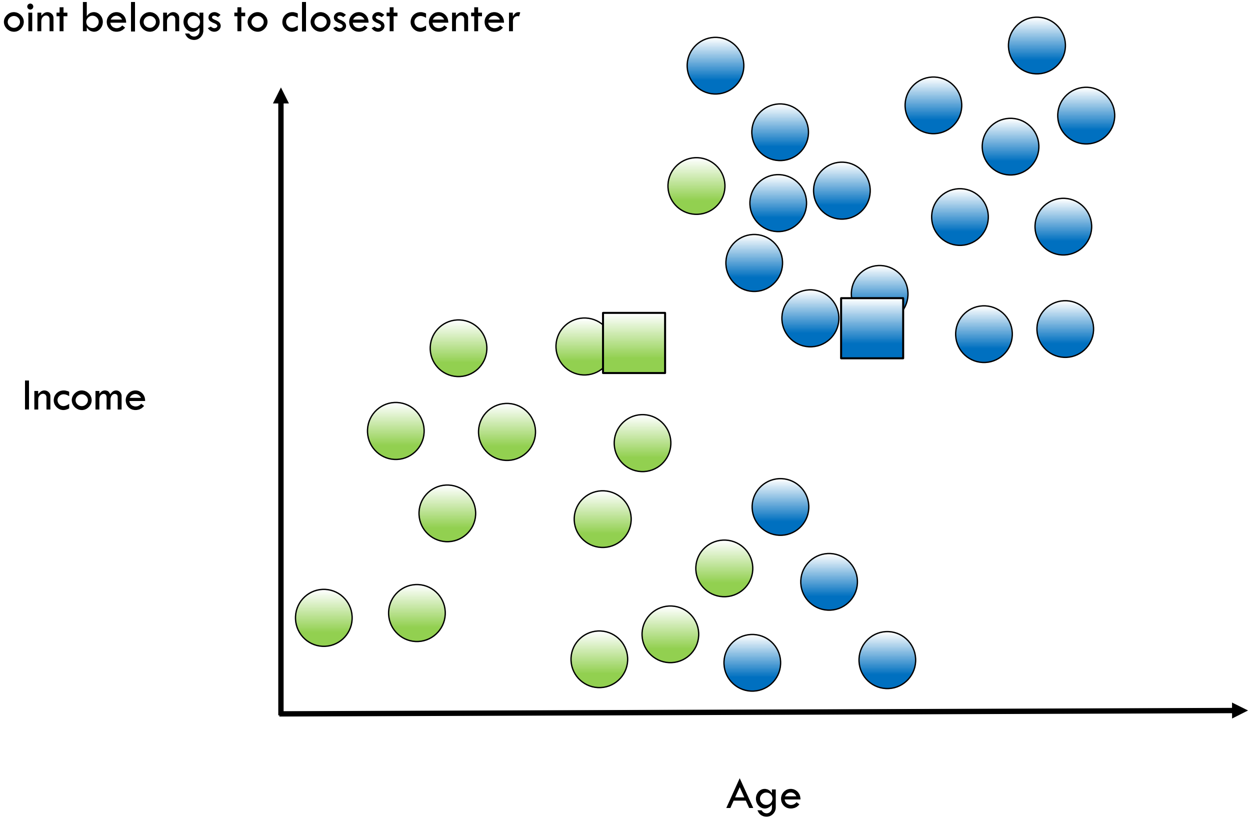

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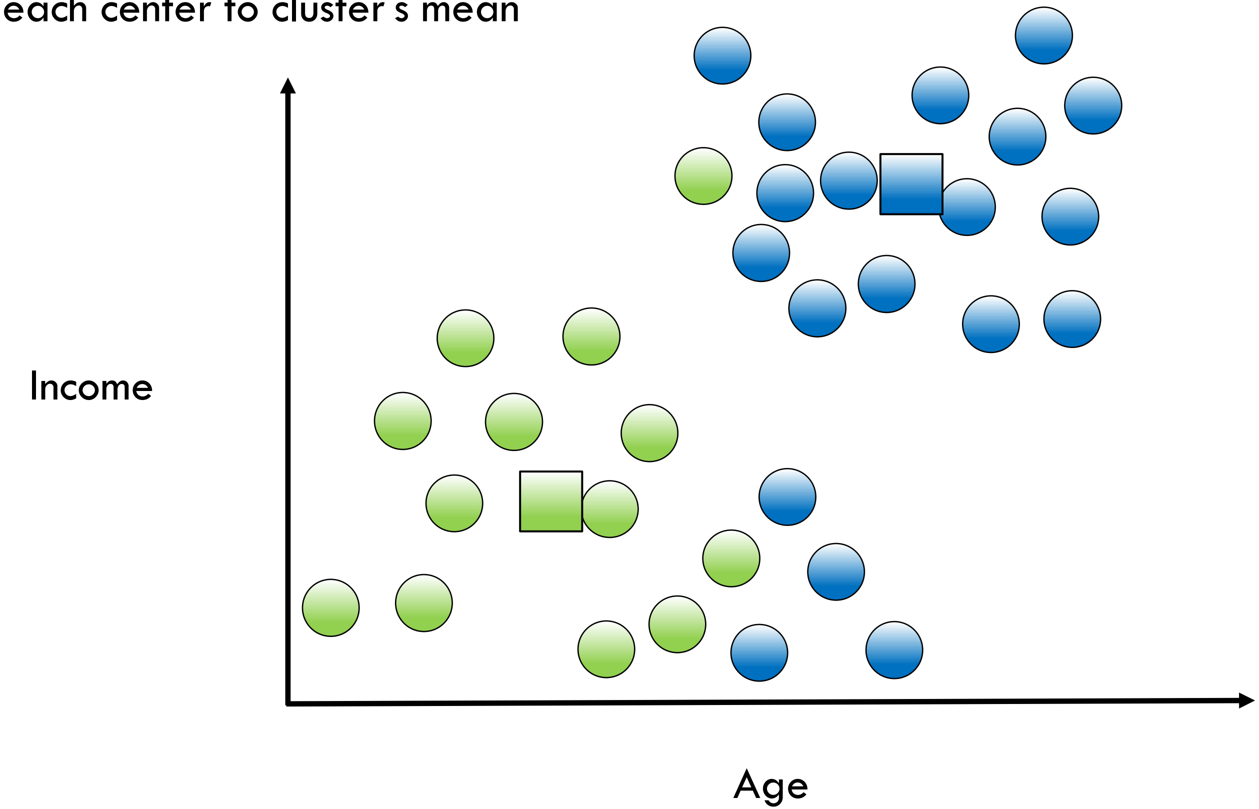
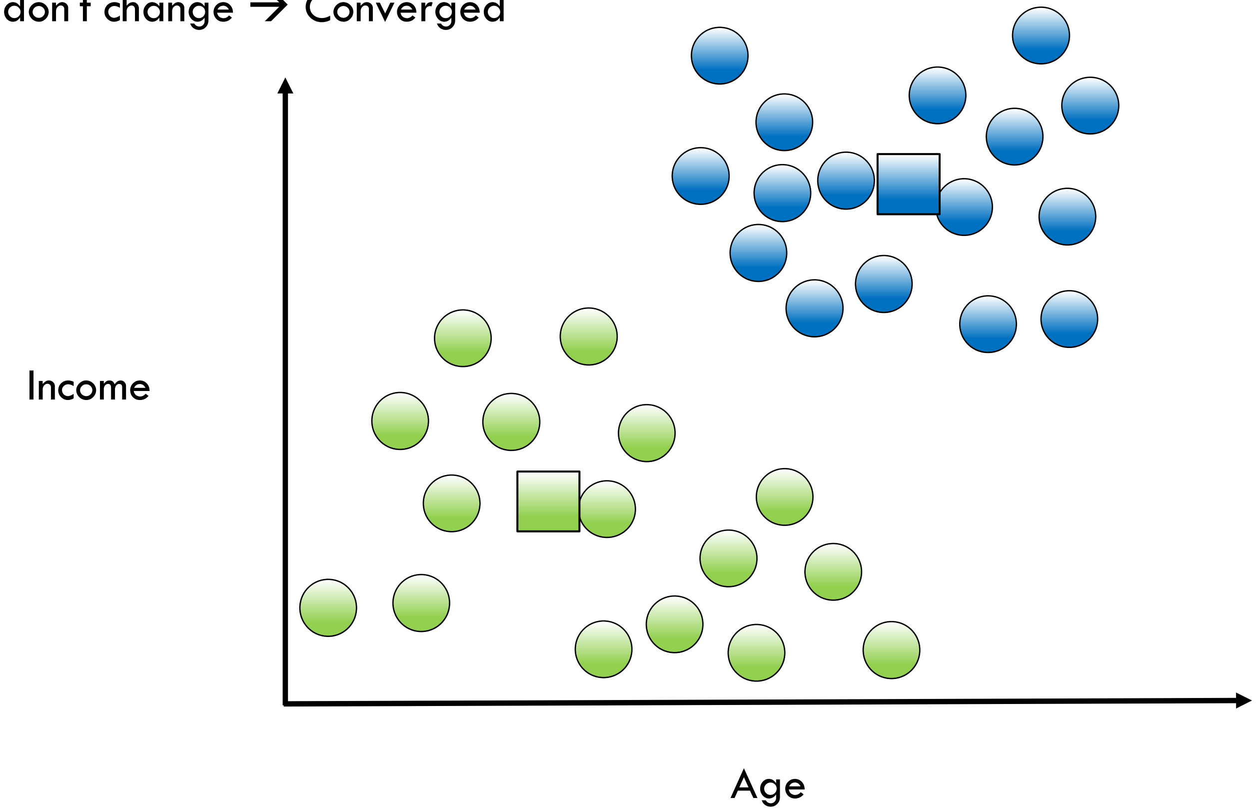


K-Means Algorithm

K = 2, Points don't change → Converged



K-Means Algorithm

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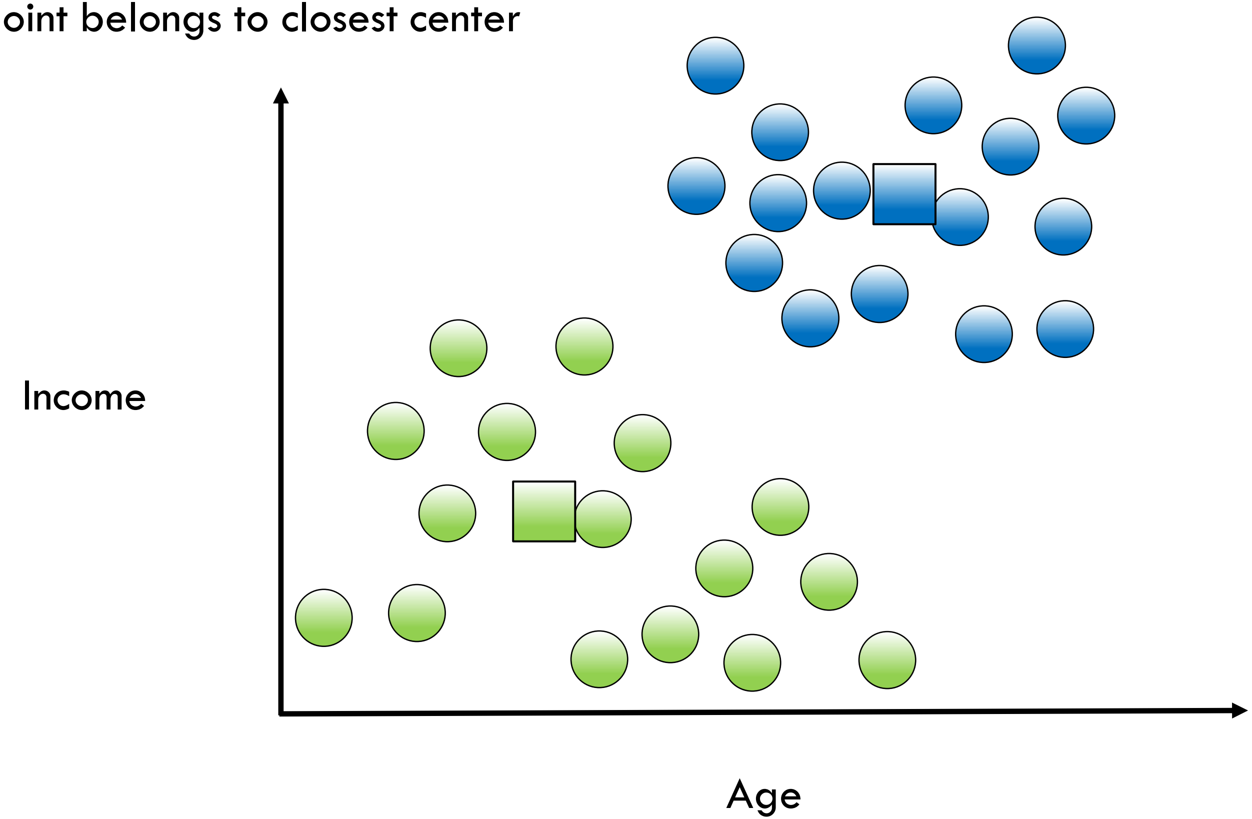
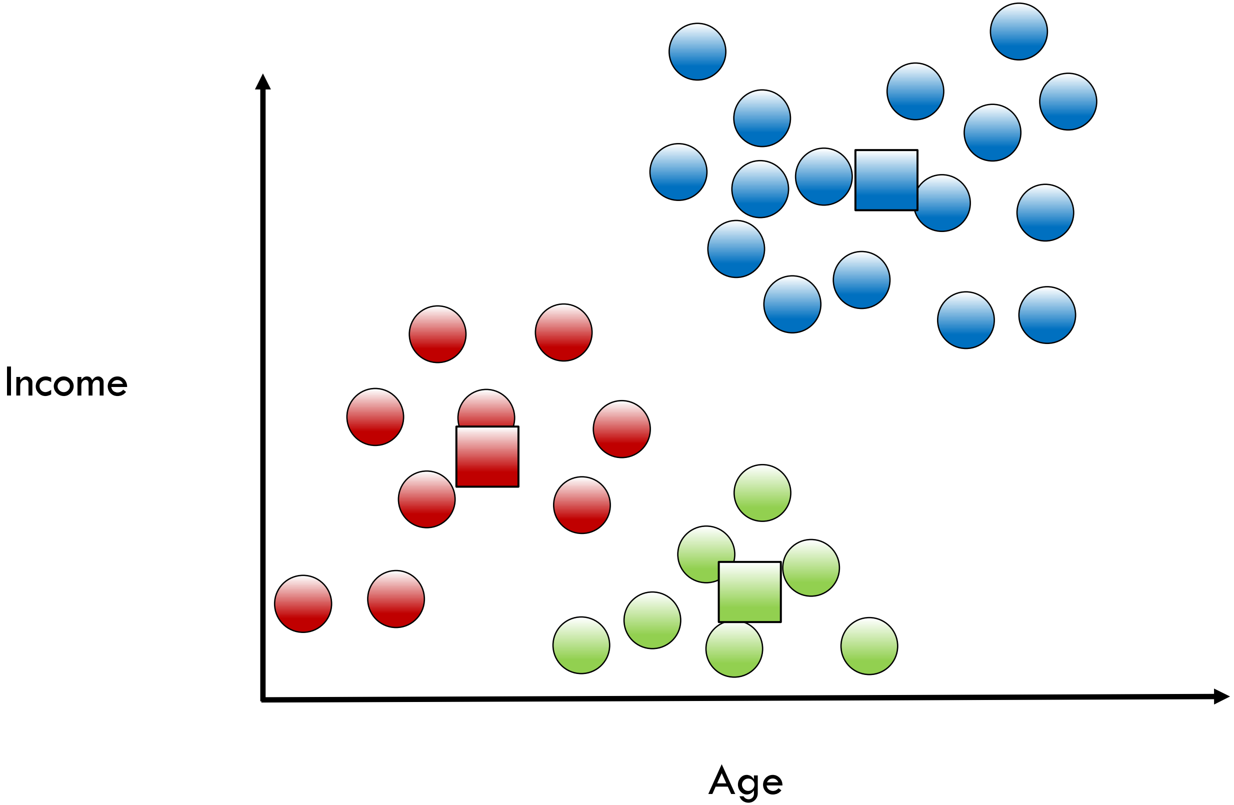


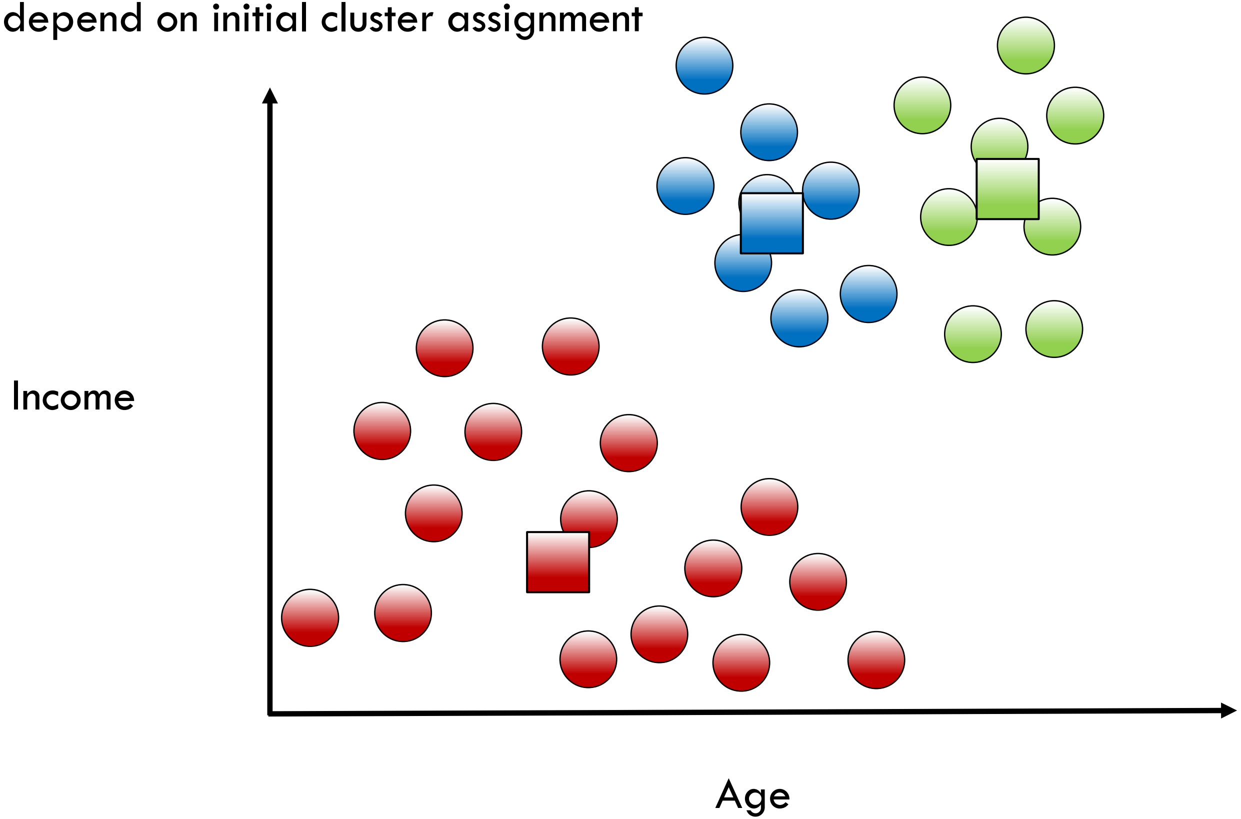
K-Means Algorithm

K = 3

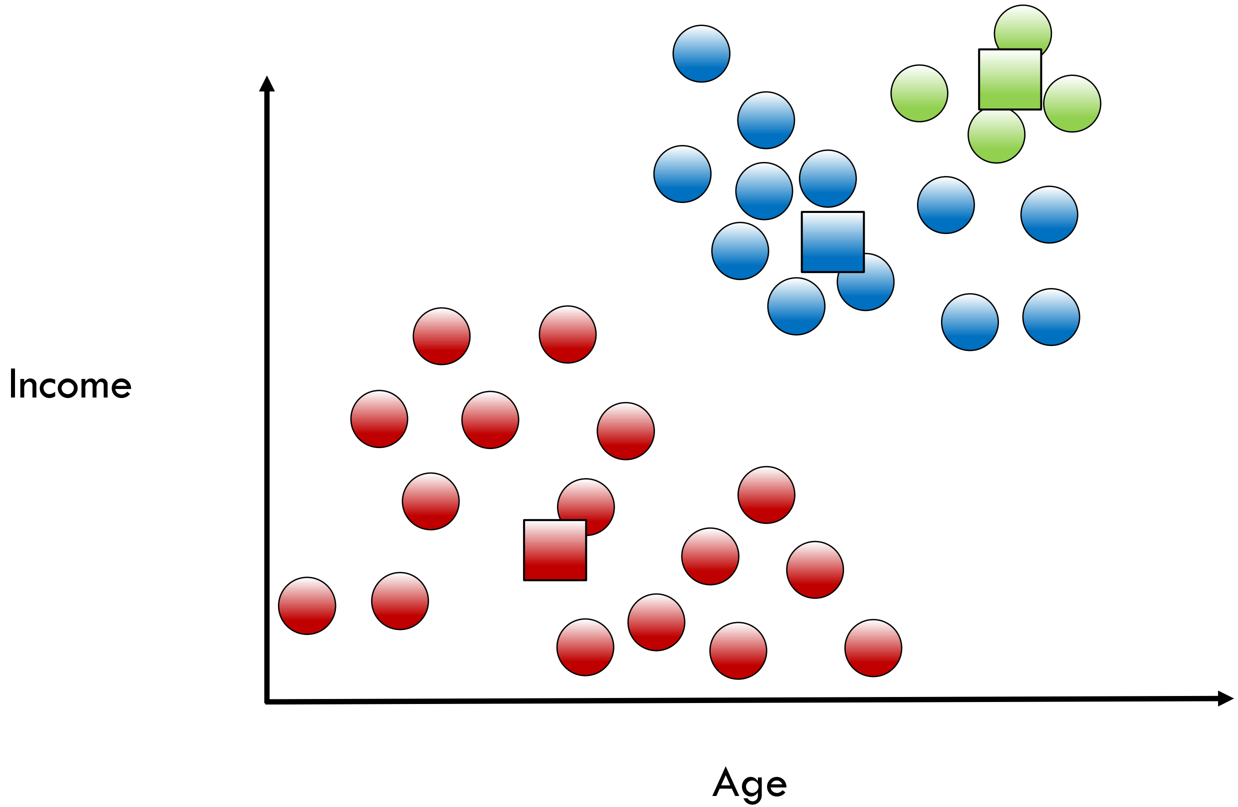


K-Means Algorithm

K = 3, Results depend on initial cluster assignment



Which Model is the Right One?



Which Model is the Right One?

- **Inertia:** sum of squared distance from each point (x_i) to its cluster (C_k)

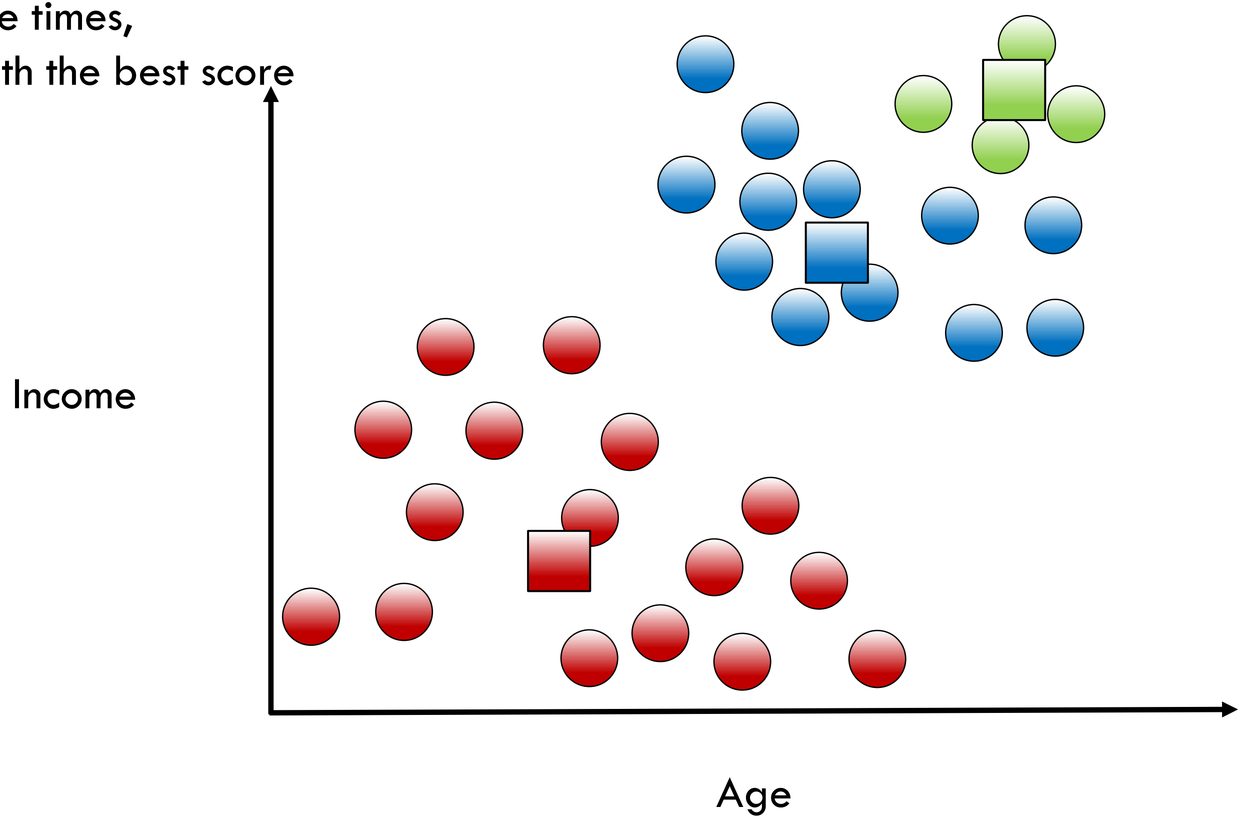
$$\sum_{i=1}^{n}(x_i - C_k)^2$$

- Smaller value corresponds to tighter clusters

- Other metrics can also be used

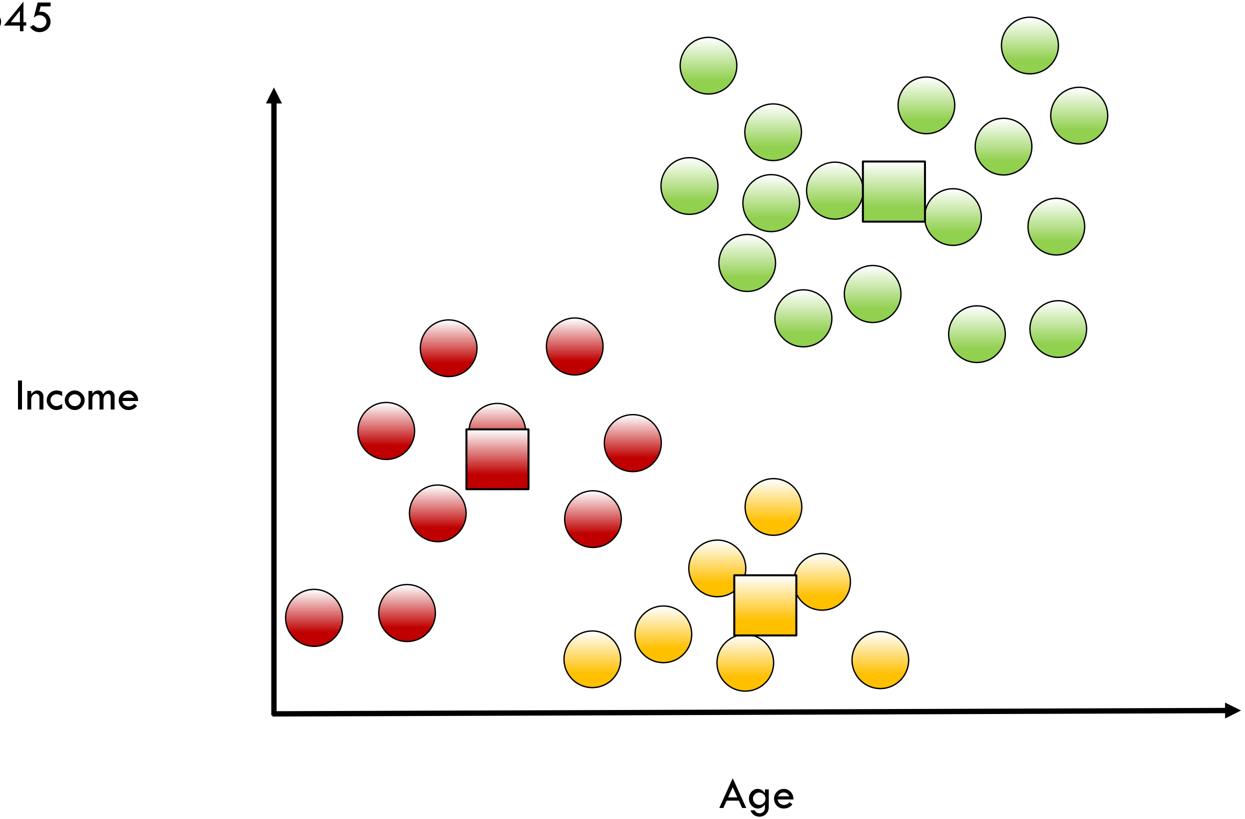
Which Model is the Right One?

Initiate multiple times,
take model with the best score



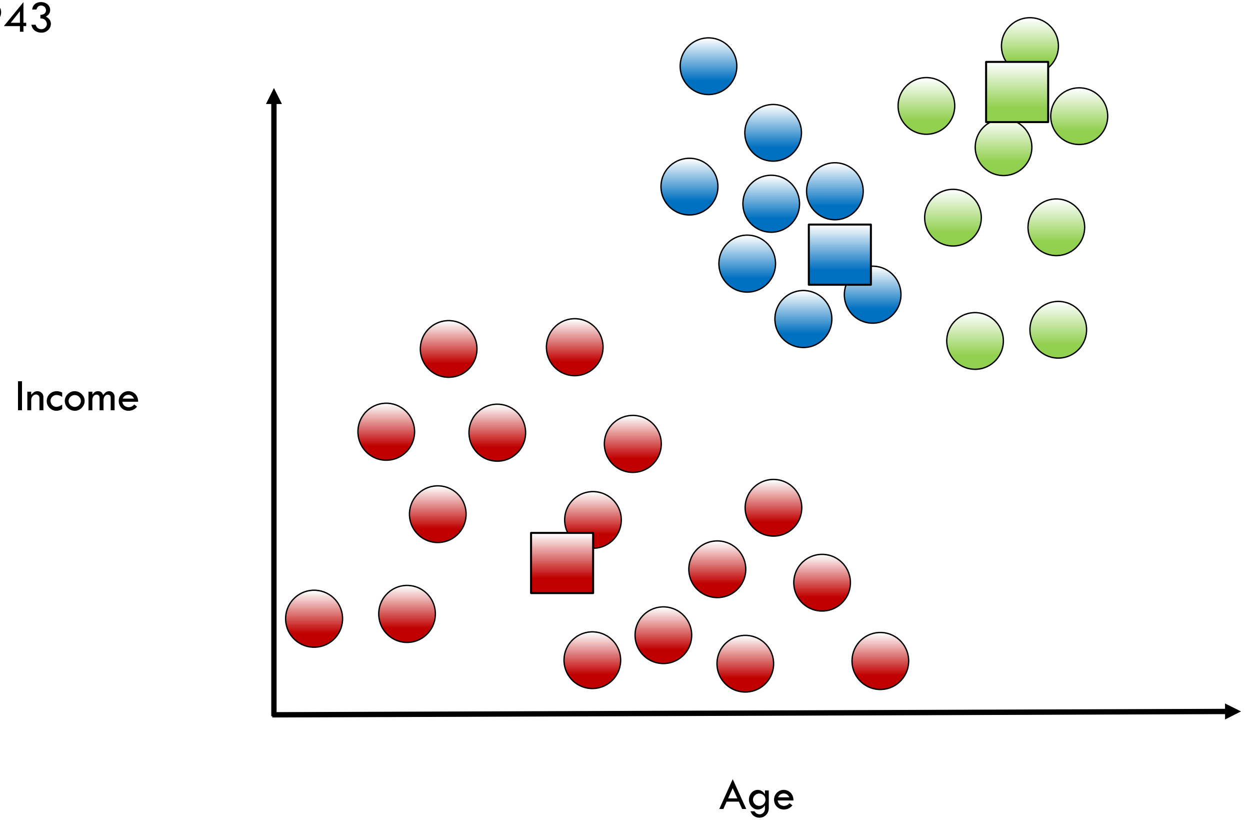
Which Model is the Right One?

Inertia = 12.645



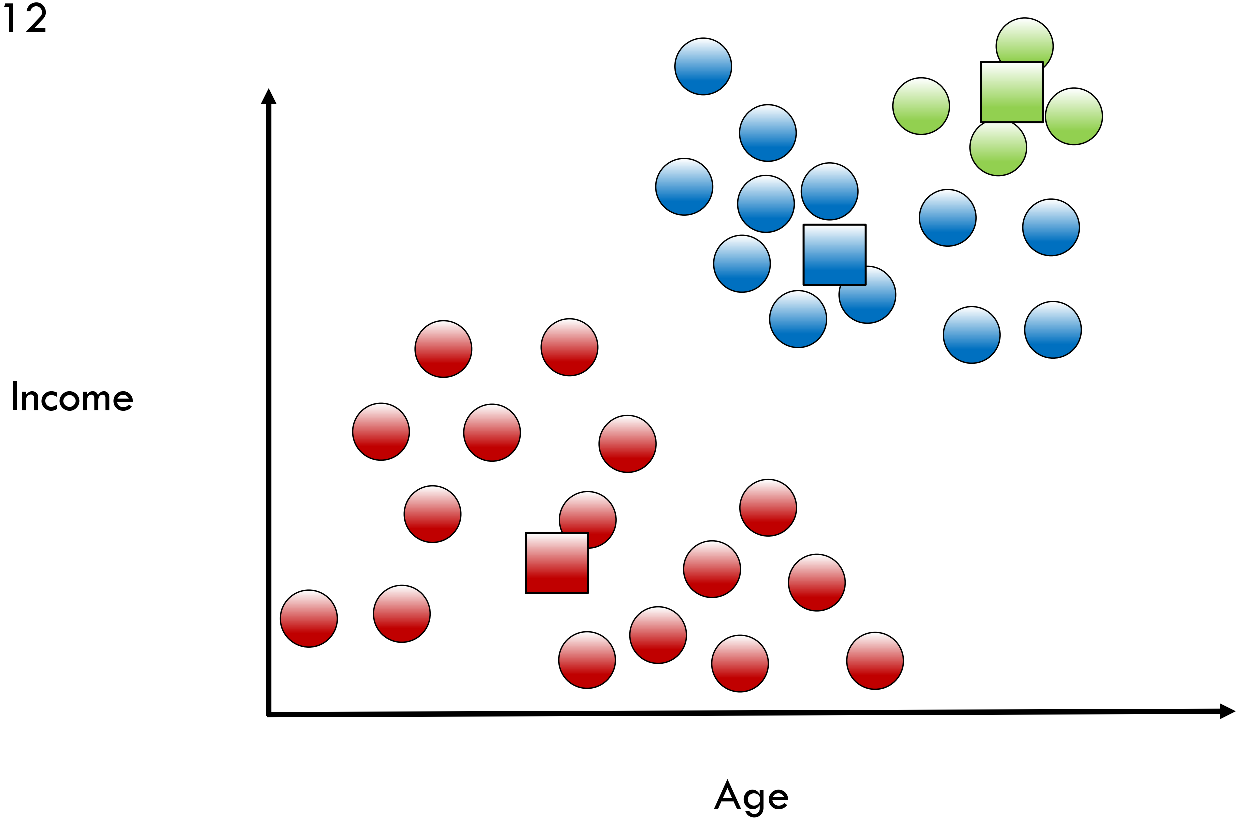
Which Model is the Right One?

Inertia = 12.943

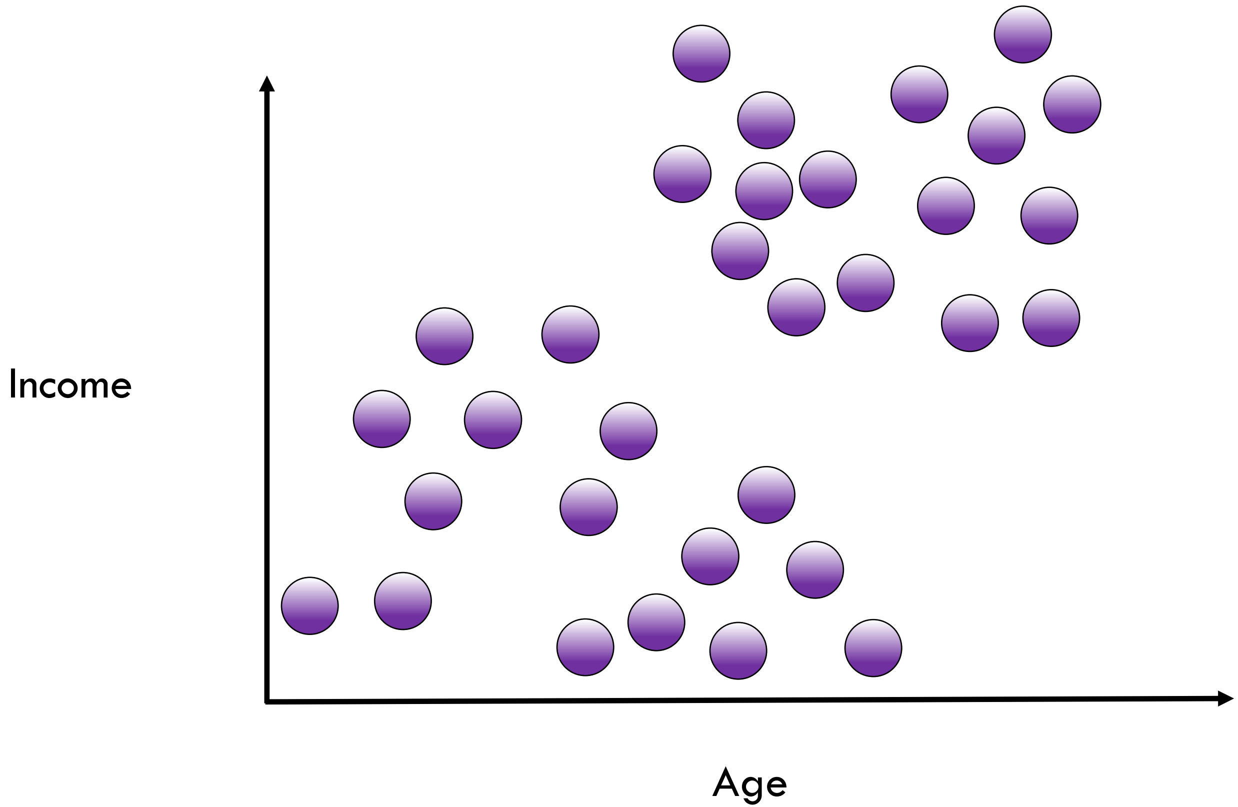


Which Model is the Right One?

Inertia = 13.112

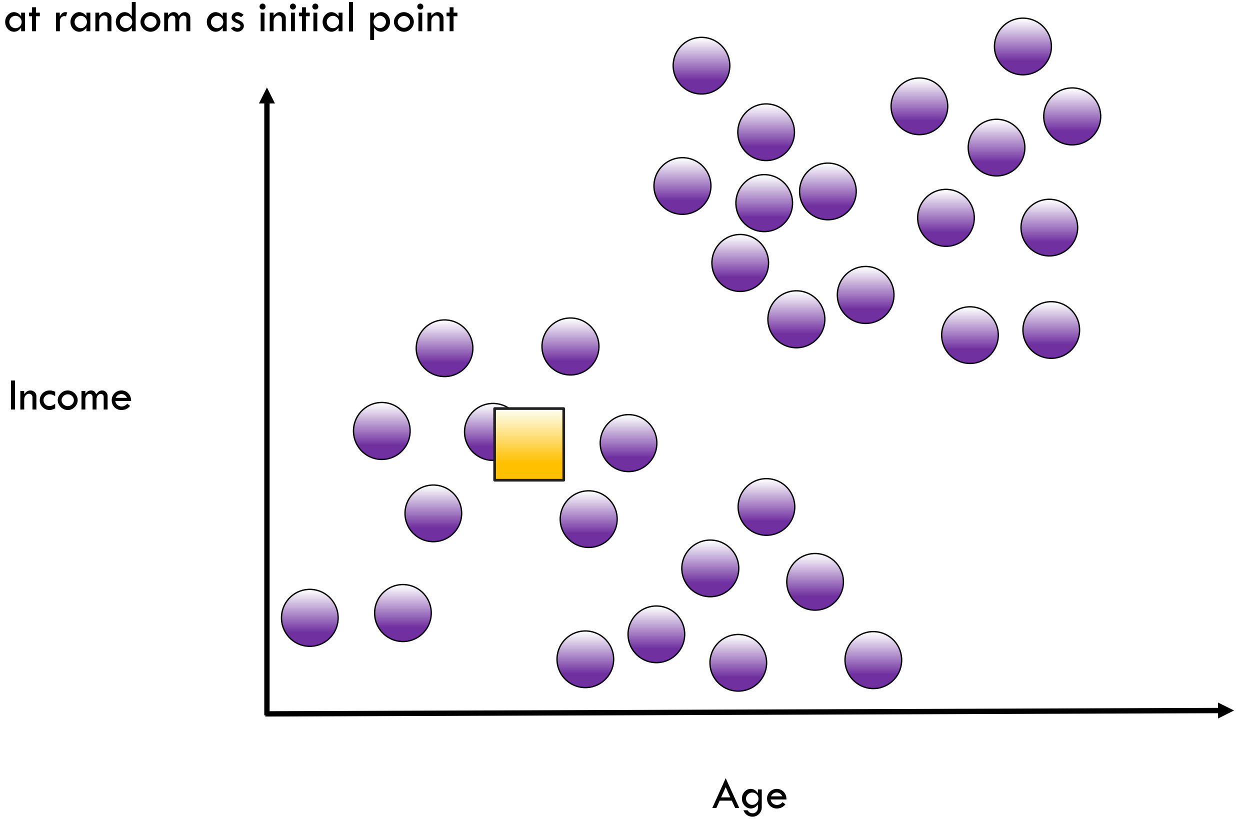


Smarter Initialization of K-Means Clusters



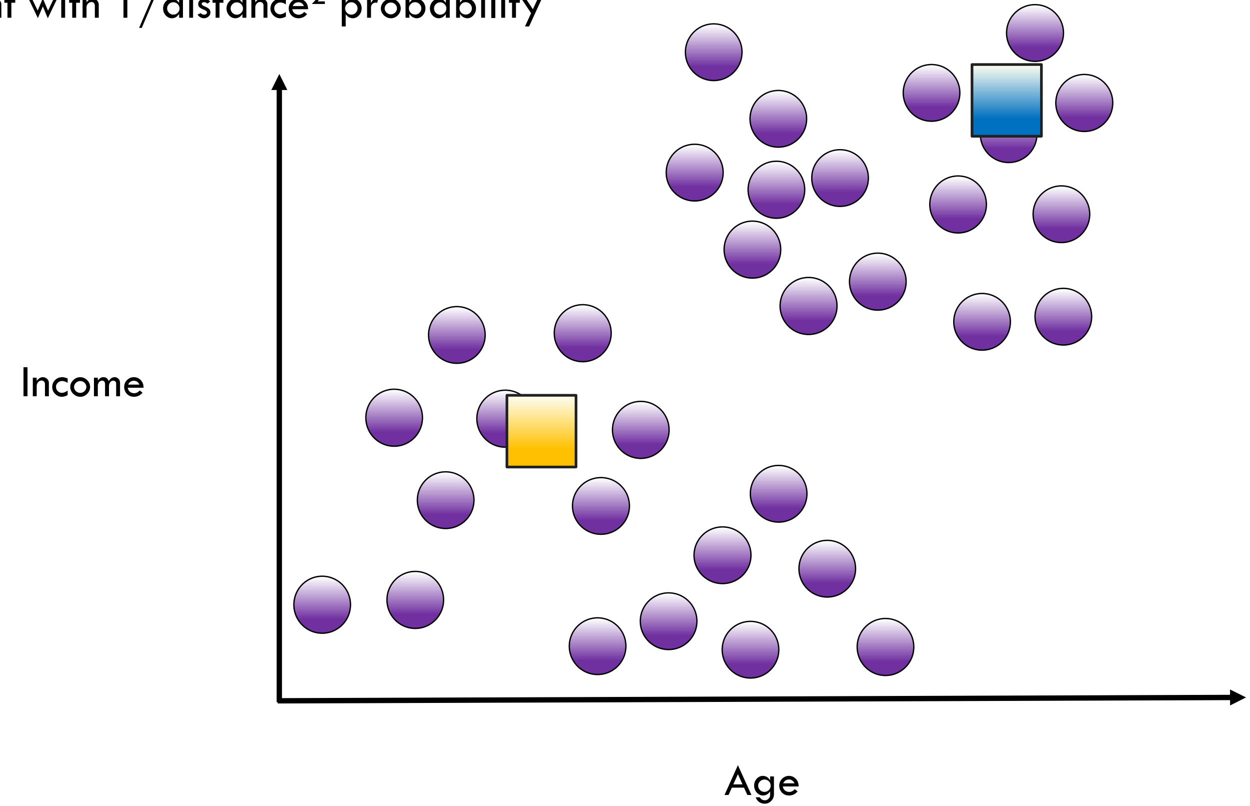
Smarter Initialization of K-Means Clusters

Pick one point at random as initial point



Smarter Initialization of K-Means Clusters

Pick next point with 1/distance^2 probability



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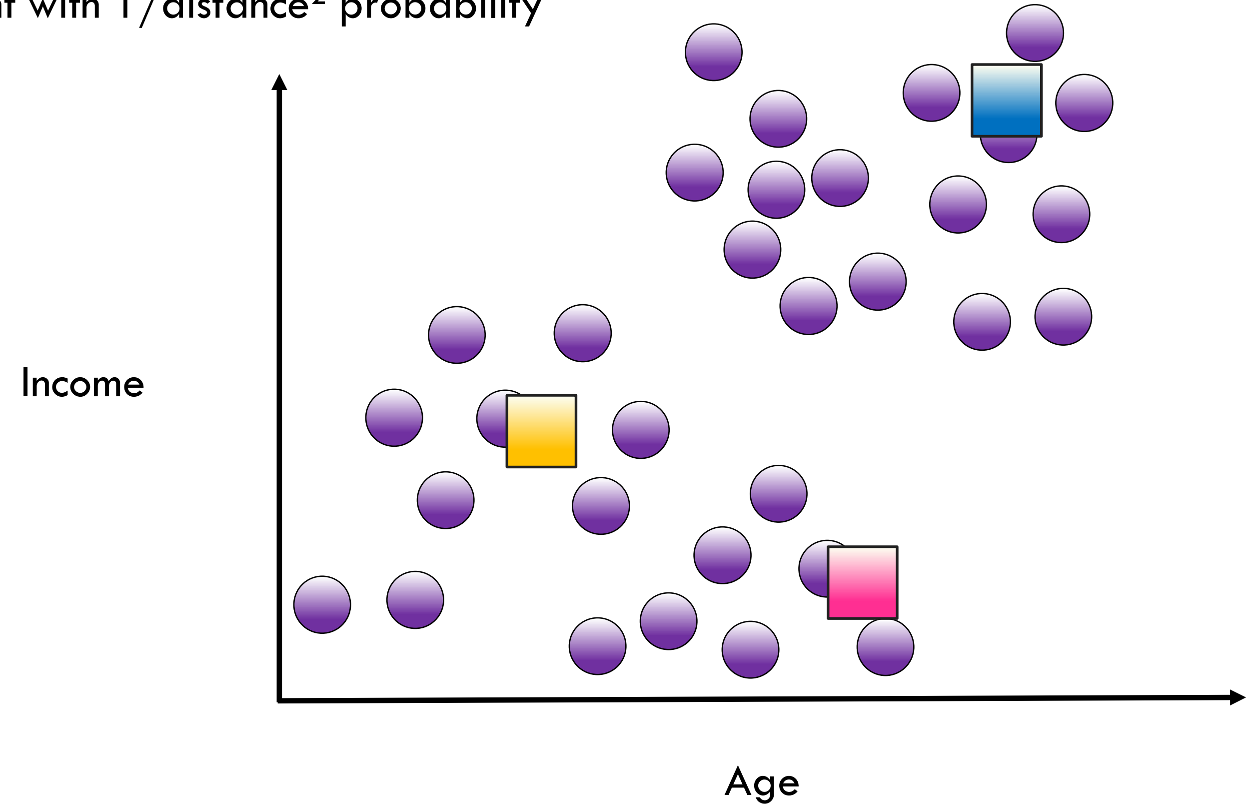
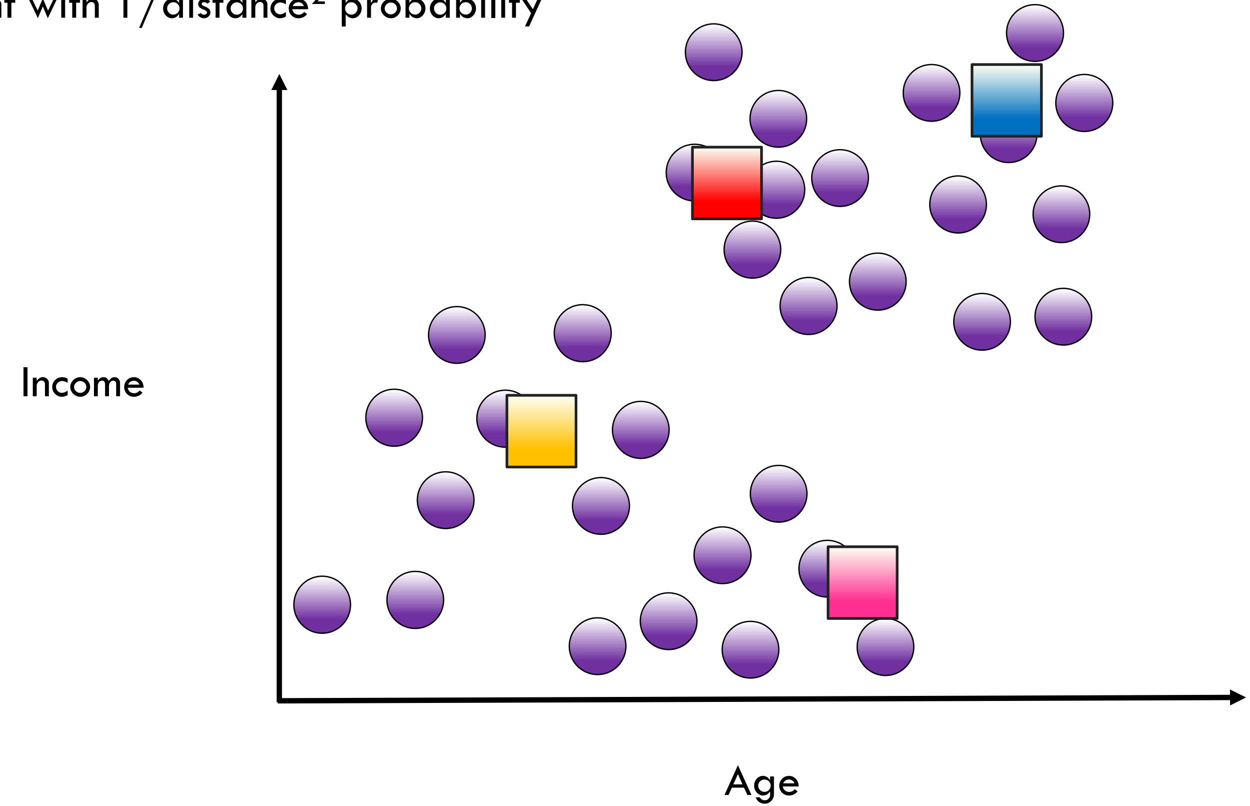


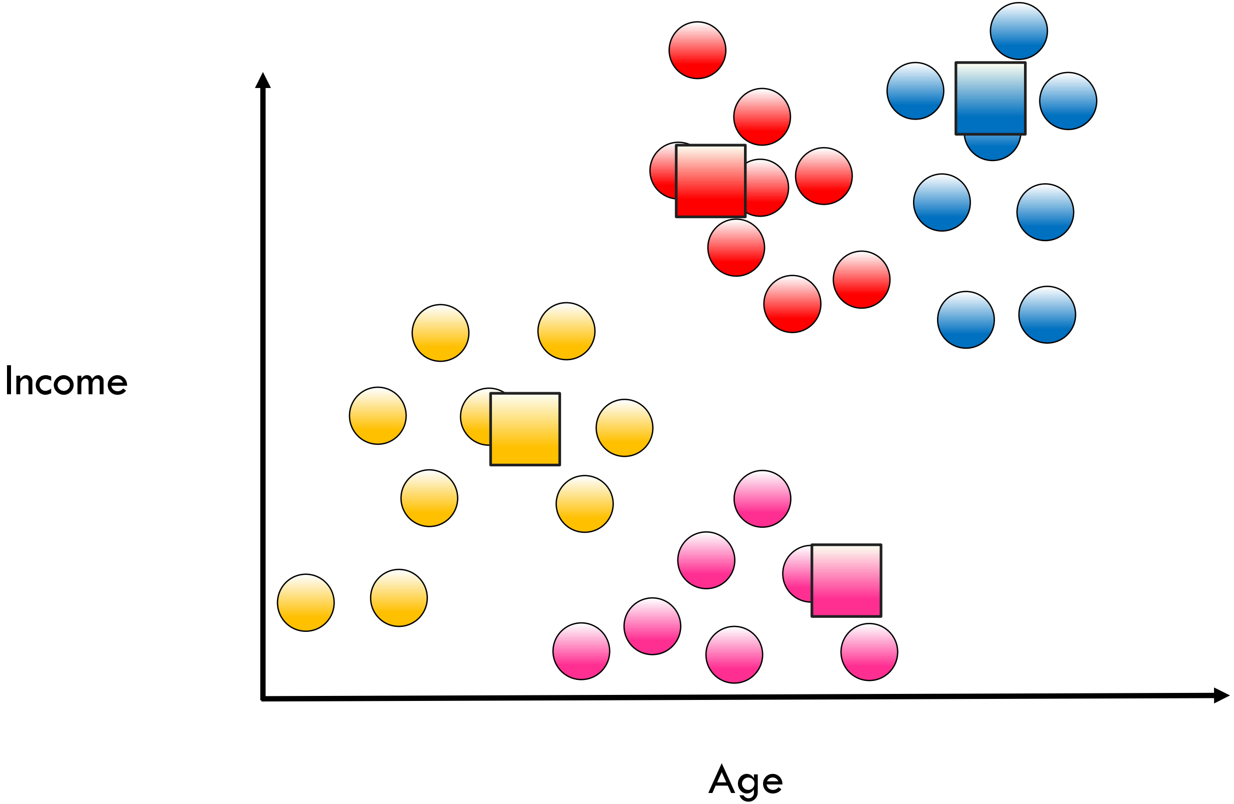
Smarter Initialization of K-Means Clusters

Pick next point with $1/\text{distance}^2$ probability



Smarter Initialization of K-Means Clusters

Assign clusters



Choosing the Right Number of Clusters

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- Sometimes the question has a K

Choosing the Right Number of Clusters

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- Clustering similar jobs on 4 CPU cores (K=4)

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- A clothing design in 10 different sizes to cover most people (K=10)

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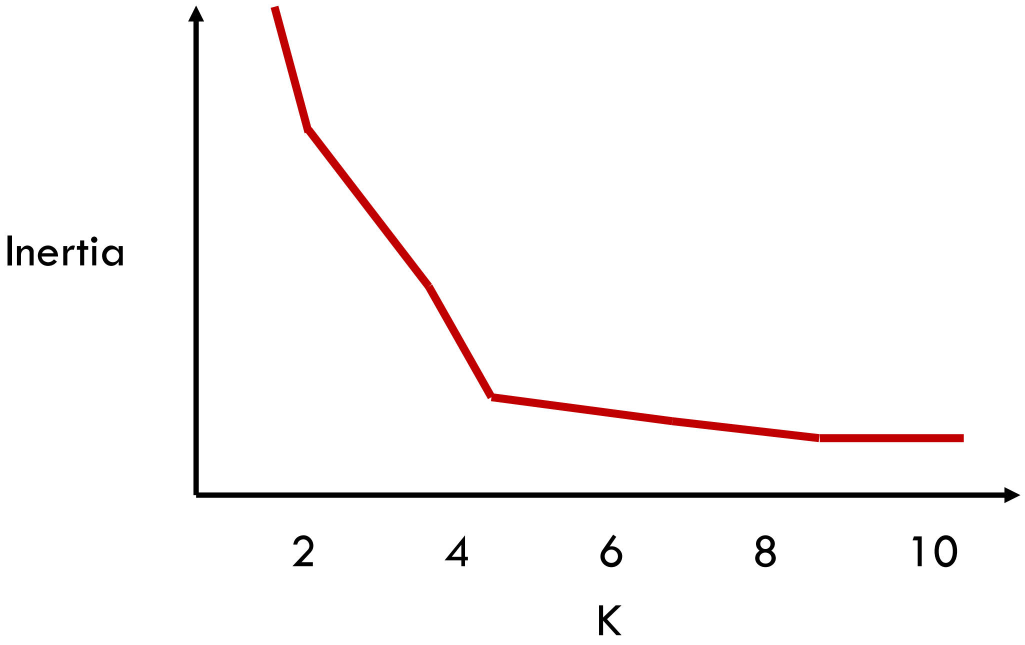
- Sometimes the question has a K
- Clustering similar jobs on 4 CPU cores (K=4)
- A clothing design in 10 different sizes to cover most people (K=10)
- A navigation interface for browsing scientific papers with 20 disciplines (K=20)

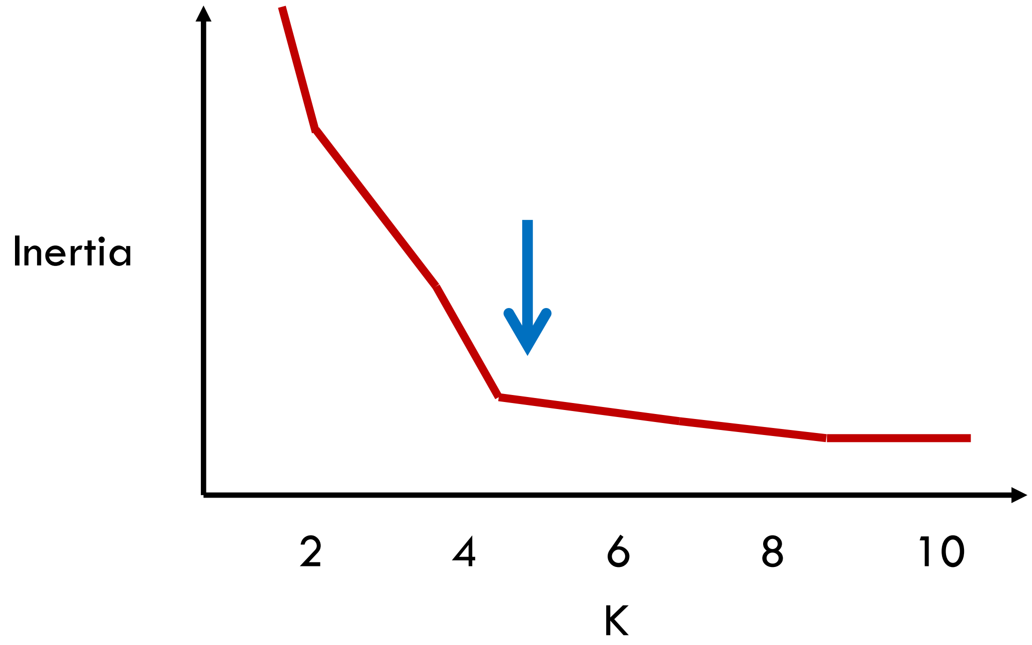
Choosing the Right Number of Clusters



- Inertia measures distance of point to cluster

r

Choosing the Right Number of Clusters



- Inertia measures distance of point to cluster
- Value decreases with increasing K as long as cluster density increases

K-Means: The Syntax

Import the class containing the clustering method

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final number of clusters

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kmeans++
cluster
initiation

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Fit the instance on the data and then predict clusters for new data

```
kmeans = kmeans.fit(X1)
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Fit the instance on the data and then predict clusters for new data

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kmeans = kmeans.fit(X1)

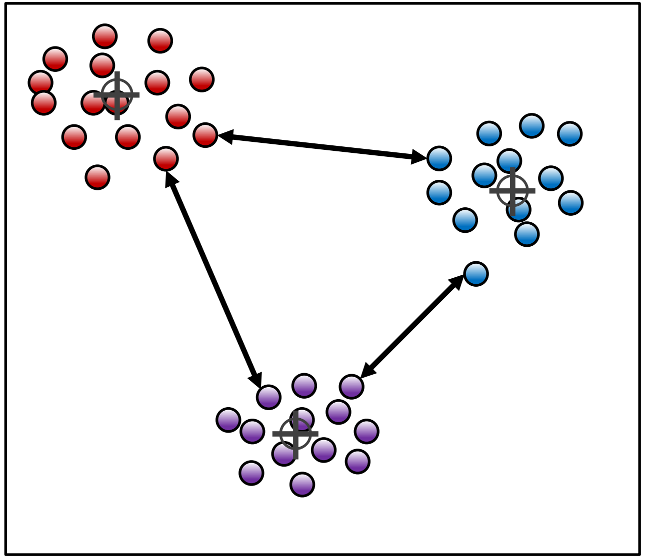
y_predict = kmeans.predict(X2)
```

Can also be used in batch mode with MiniBatchKMeans.

Software

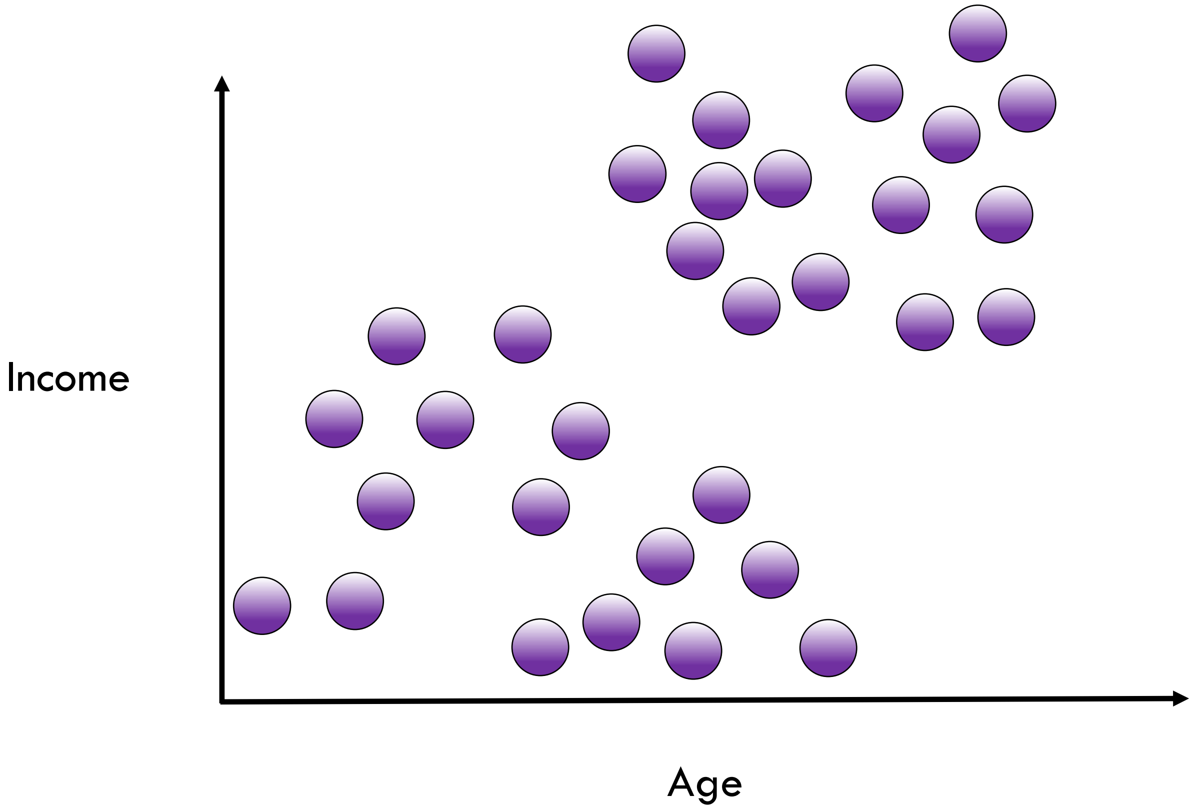
Distance Metrics

Distance Metric Choice

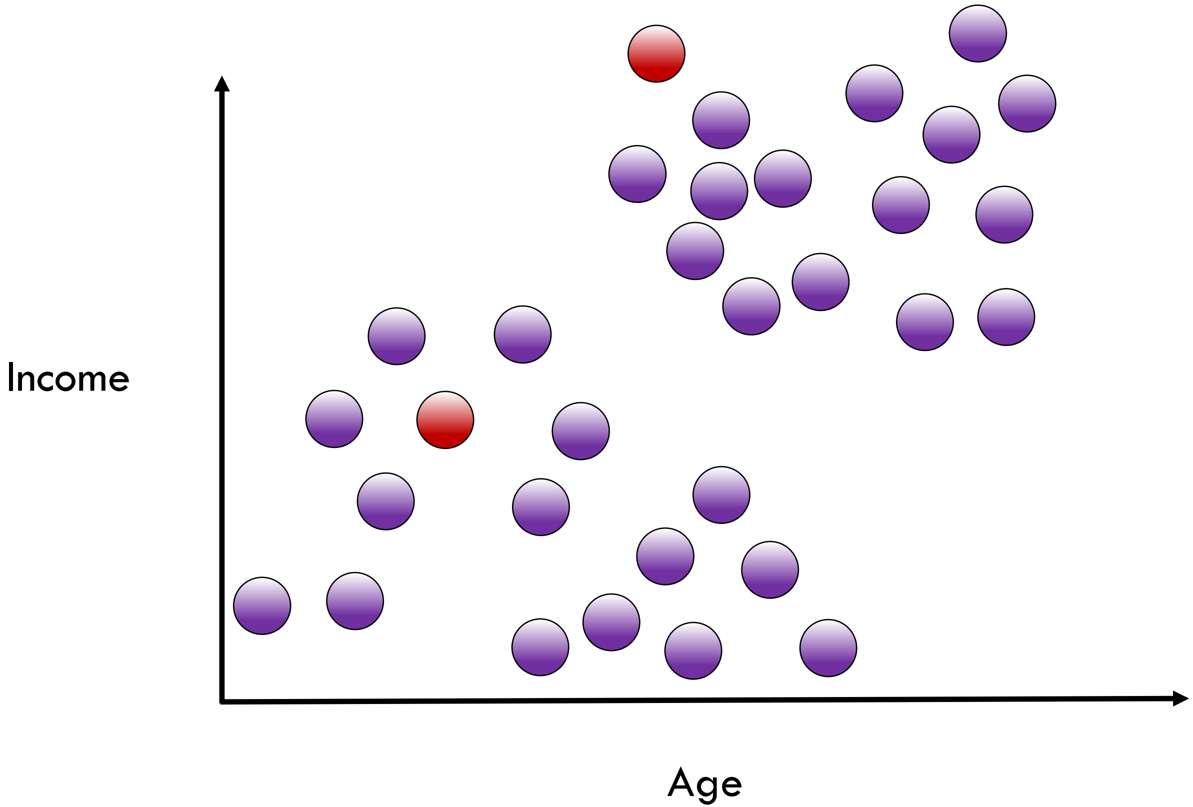


- Choice of distance metric is extremely important to clustering success
- Each metric has strengths and most appropriate use-cases…
- …but sometimes choice of distance metric is also based on empirical evaluation

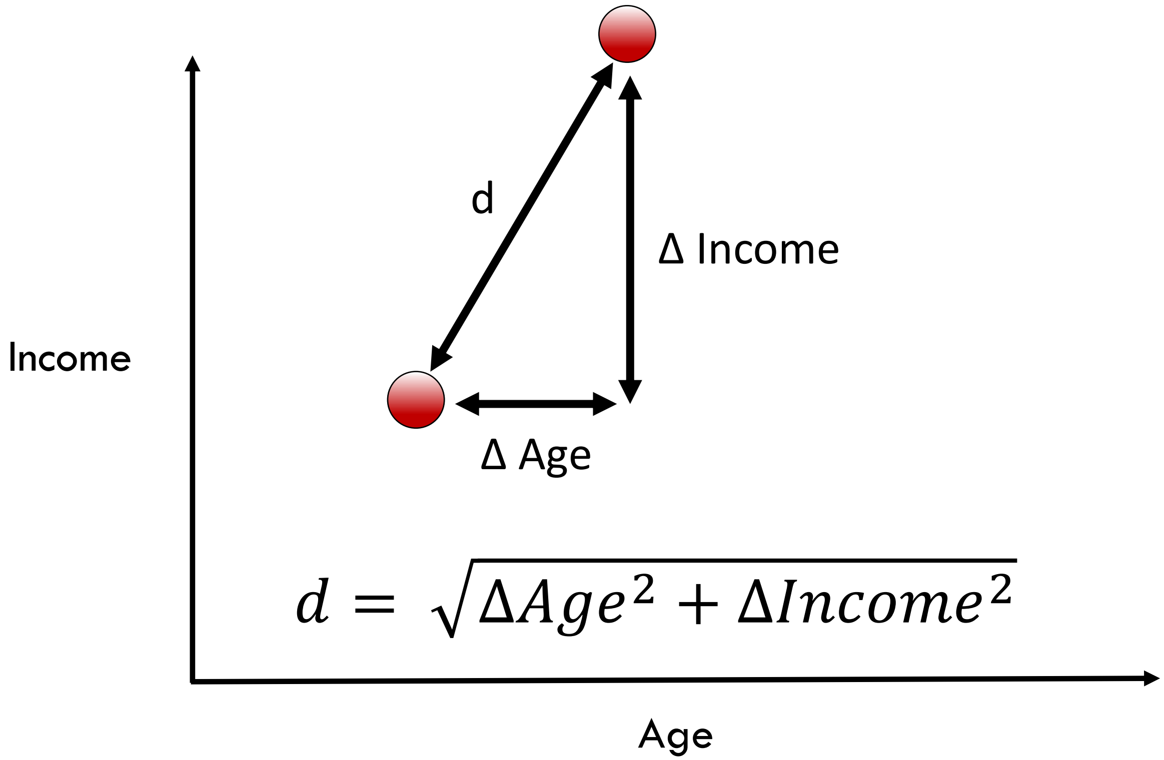
Euclidean Distance



Euclidean Distance

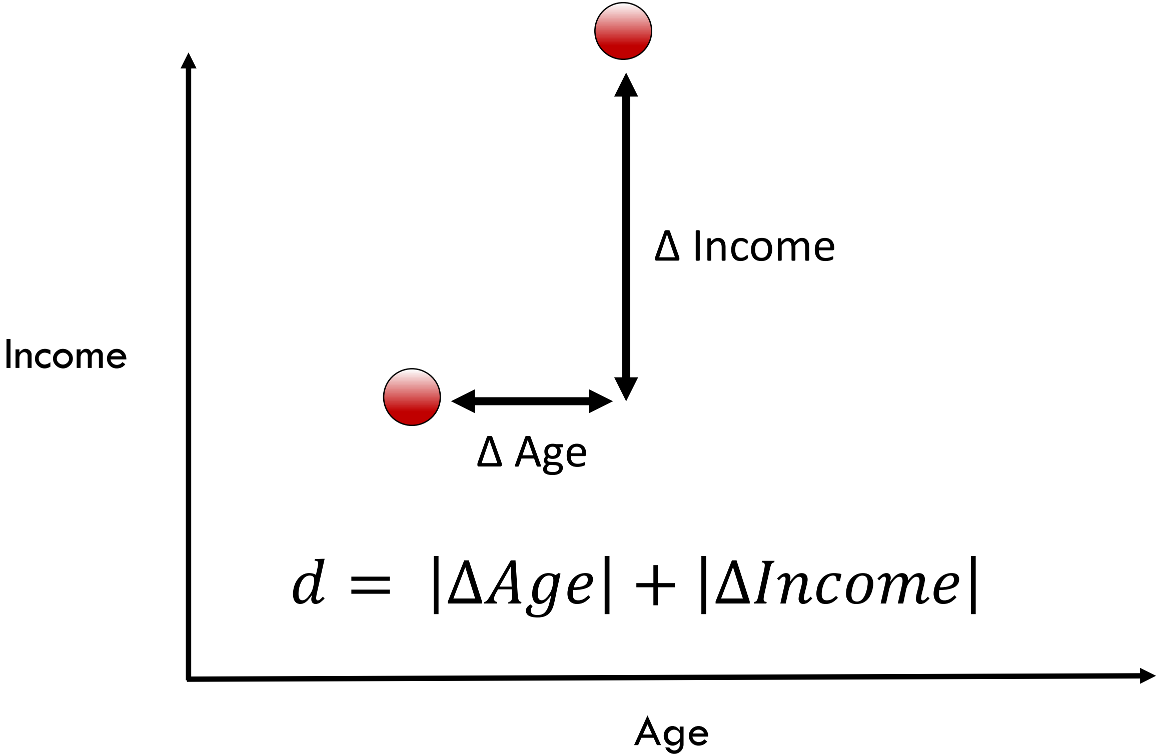


Euclidean Distance (L2 Distance)



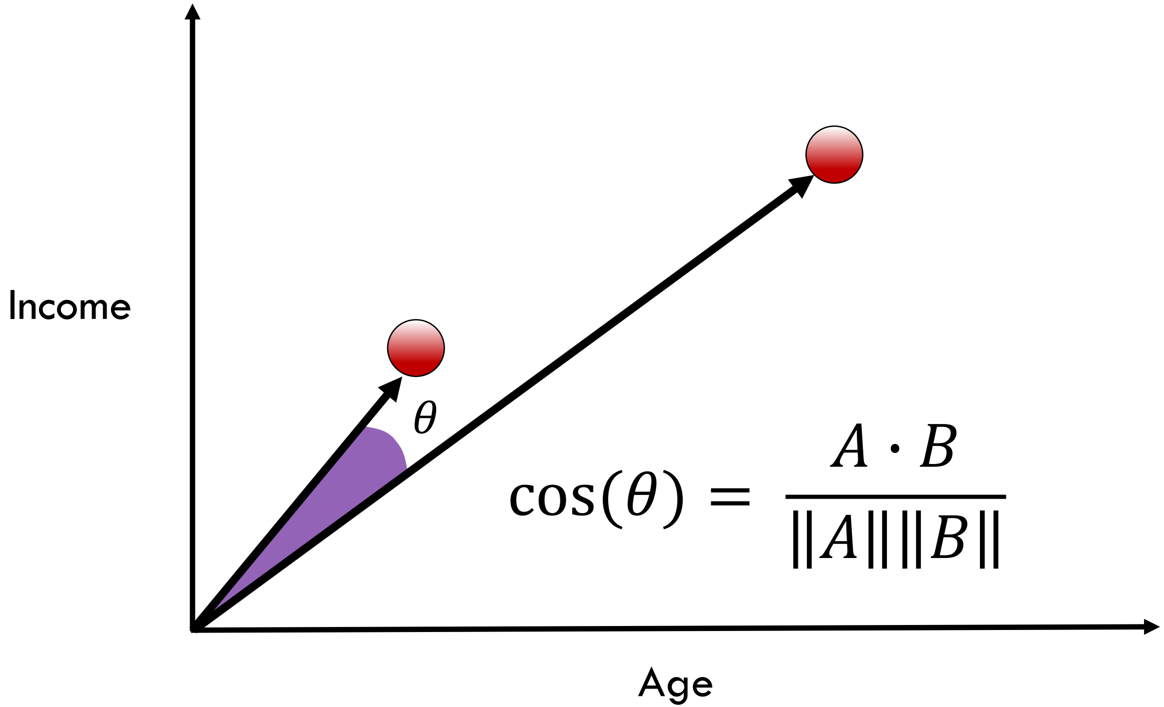
$$d = \sqrt{\Delta Age^2 + \Delta Income^2}$$

Manhattan Distance (L1 or City Block Distance)

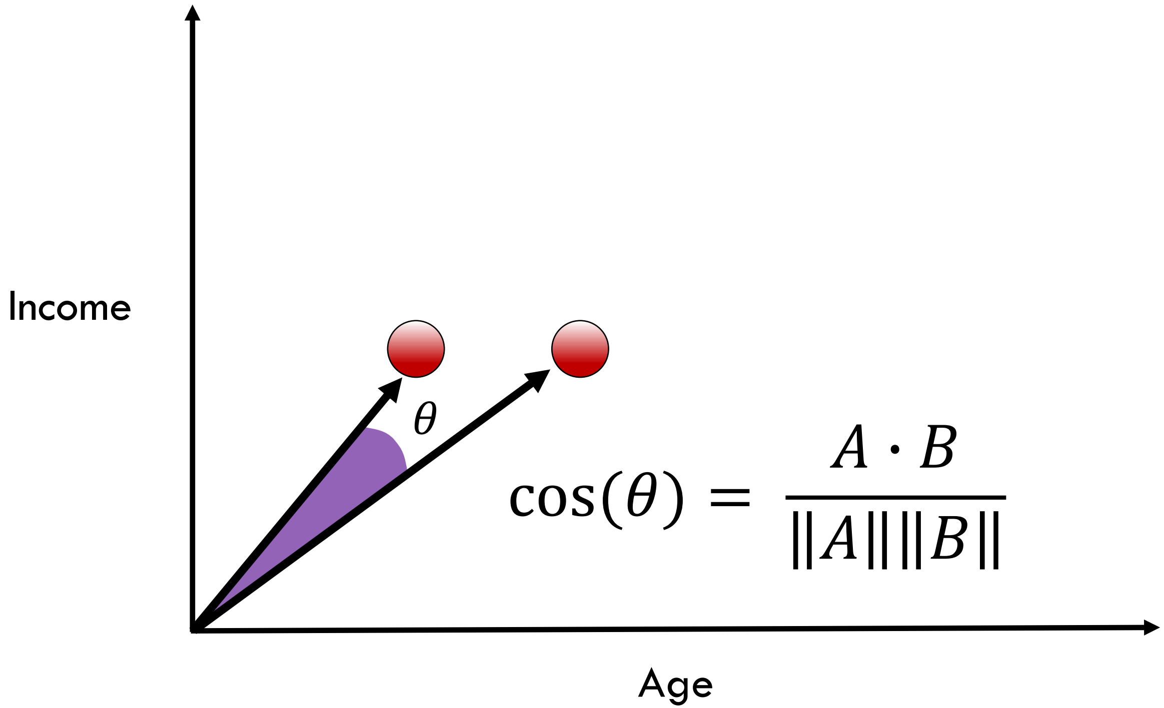


$$d = |\Delta Age| + |\Delta Income|$$

Cosine Distance



Cosine Distance



$$\cos(\theta) = \frac{A \cdot B}{\|A\|\|B\|}$$

Euclidean vs Cosine Distance

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- Euclidean distance is more sensitive to curse of dimensionality (see lesson 12)

Jaccard Distance

Applies to sets (like word occurrence)

- **Sentence A:** "I like chocolate ice cream."
- set A = {I, like, chocolate, ice, cream}
- **Sentence B:** "Do I want chocolate cream or vanilla cream?"
- set B = {Do, I, want, chocolate, cream, or, vanilla}

$$1 - \frac{A \cap B}{A \cup B} = 1 - \frac{len(shared)}{len(unique)}$$

Jaccard Distance

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$$1 - \frac{A \cap B}{A \cup B} = 1 - \frac{3}{9}$$

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distance metric choice

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Other distance metric choices are: cosine, manhattan, jaccard, etc.

Distance metric methods can also be imported specifically, e.g.:

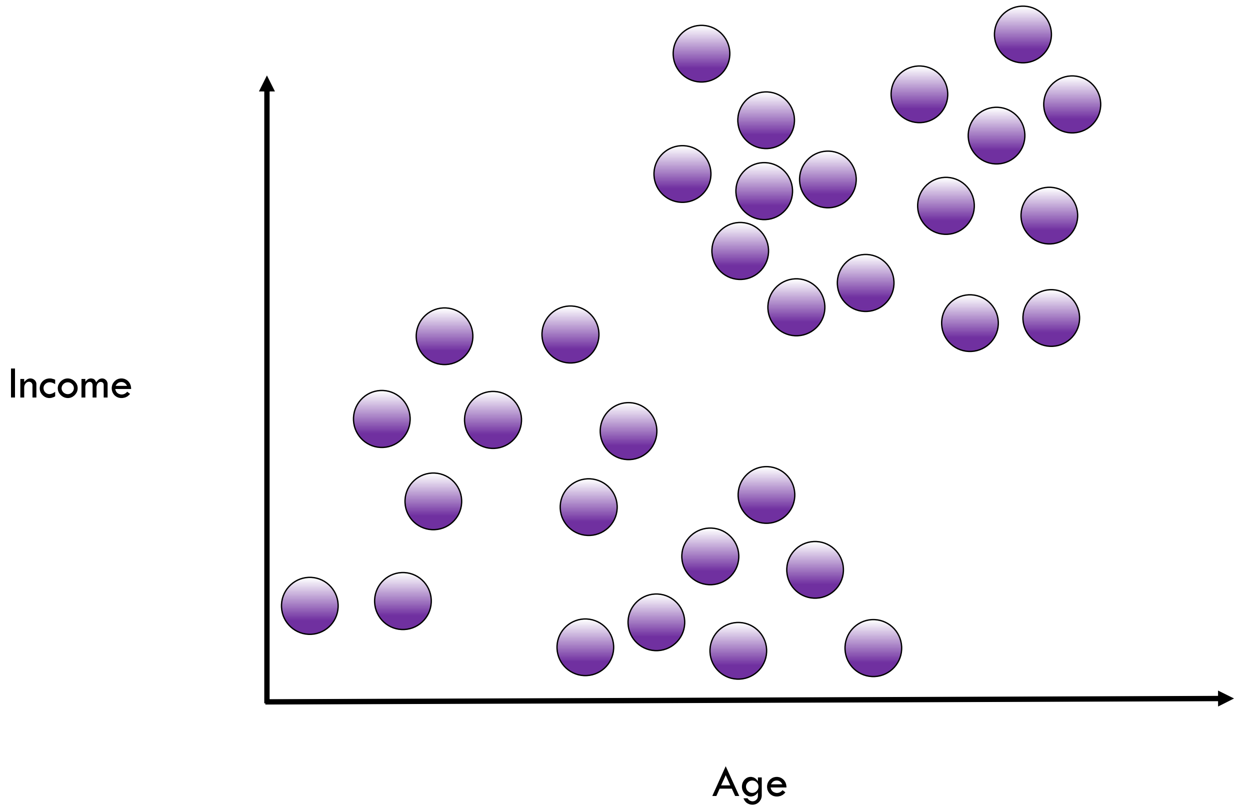
```
from sklearn.metrics import euclidean_distances
```

Software

Software

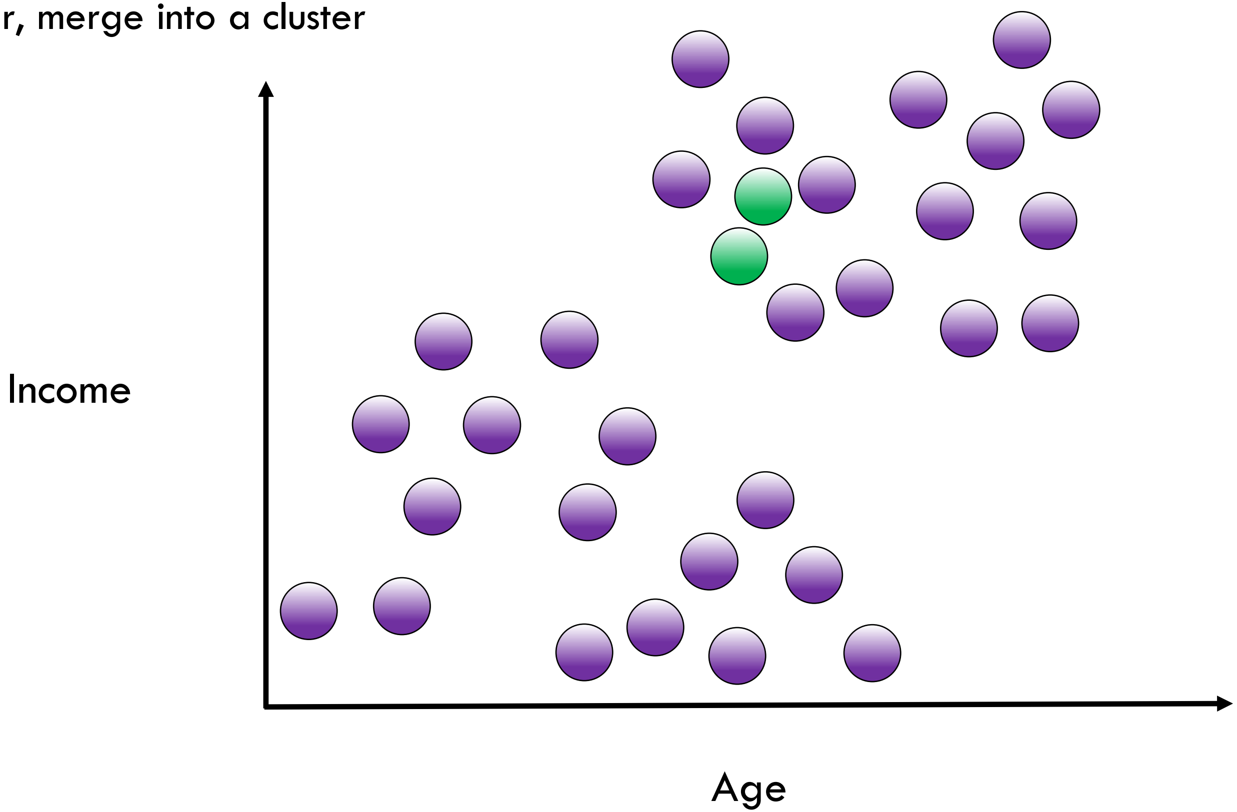
Hierarchical Agglomerative Clustering

Hierarchical Agglomerative Clustering



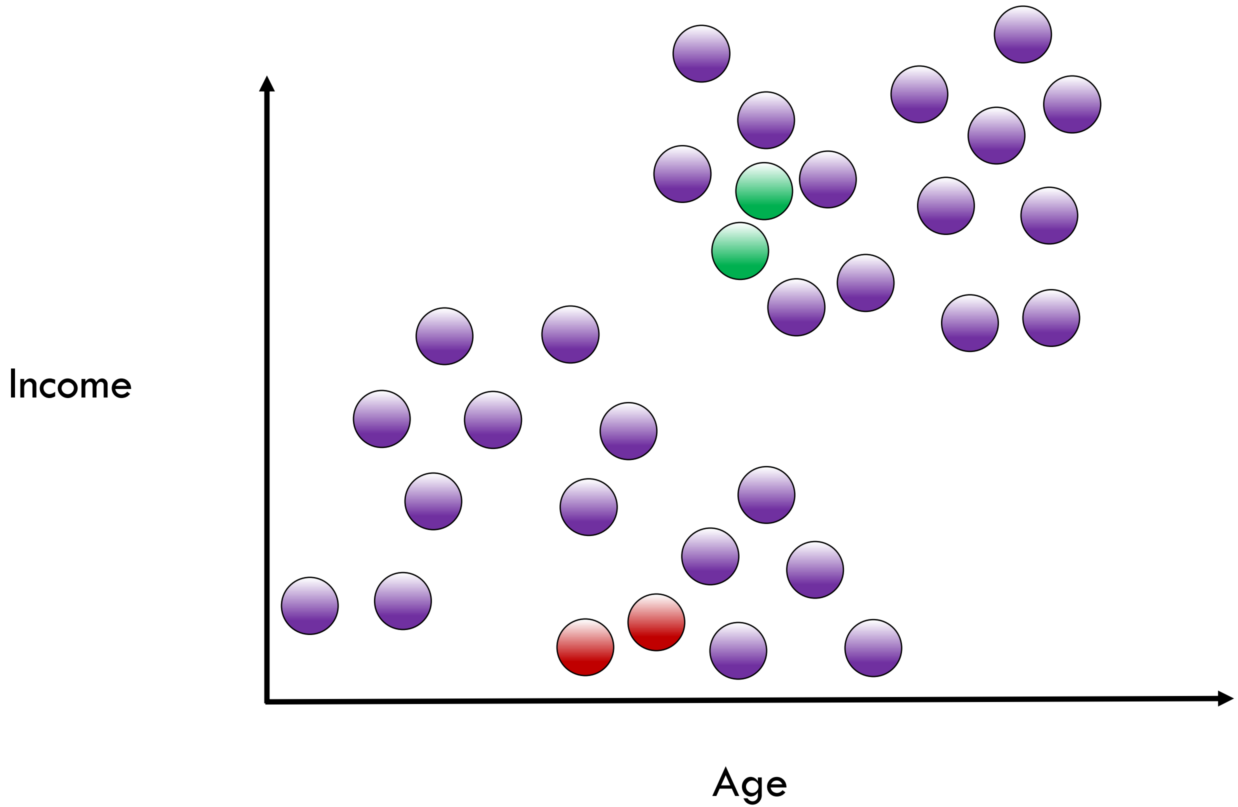
Hierarchical Agglomerative Clustering

Find closest pair, merge into a cluster



Hierarchical Agglomerative Clustering

Find next closest pair and merge



Hierarchical Agglomerative Clustering

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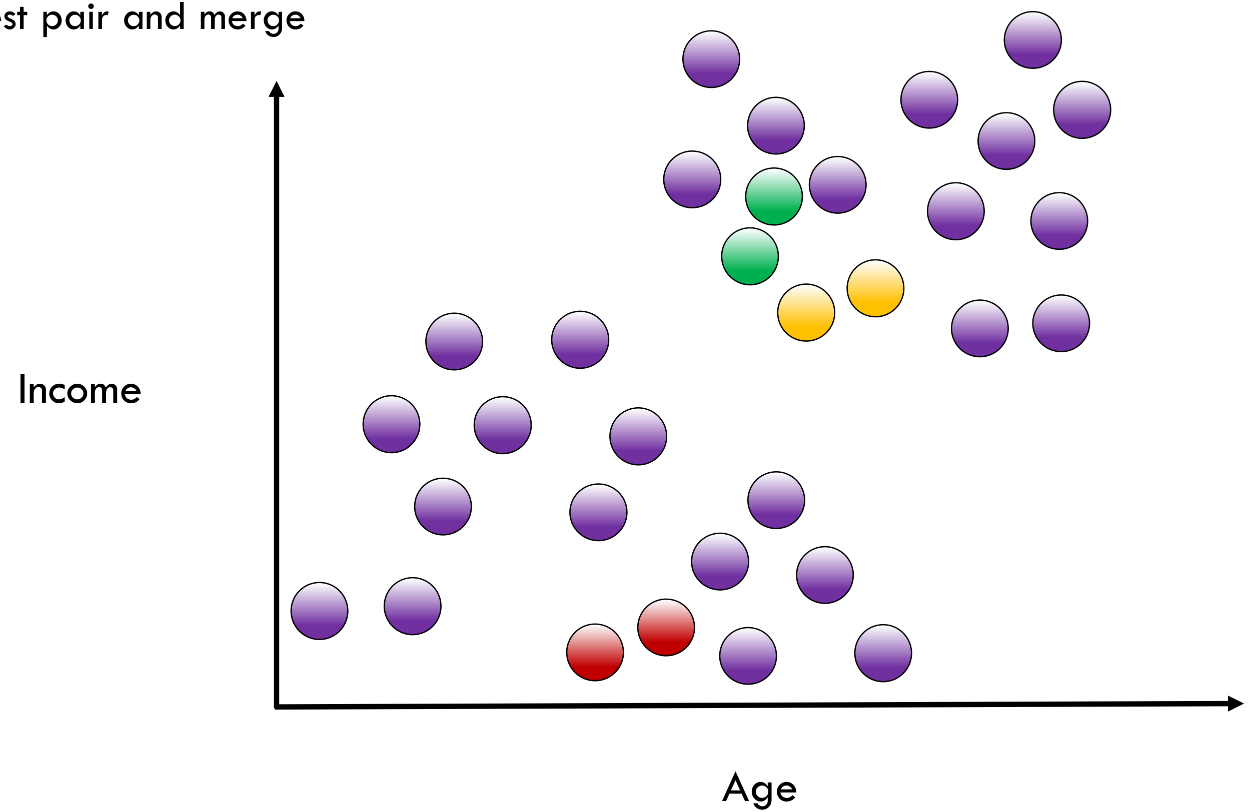
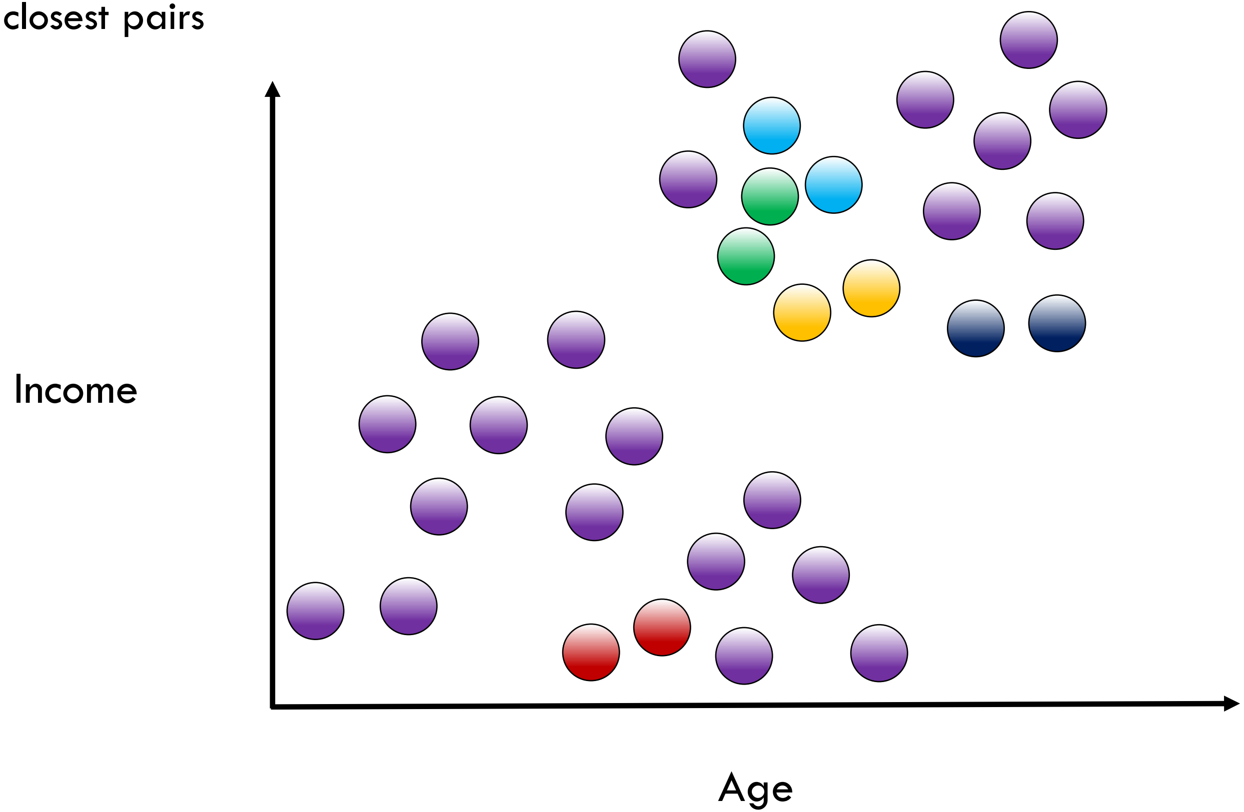


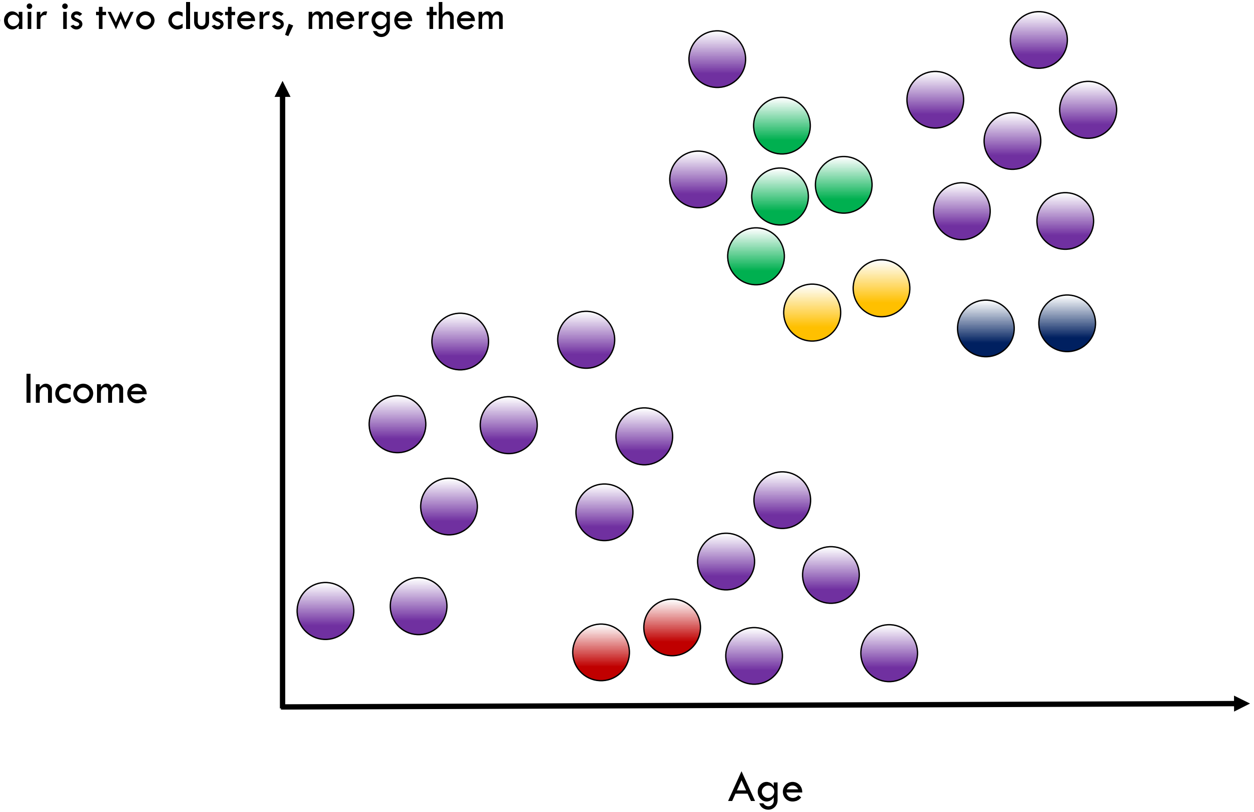
Hierarchical Agglomerative Clustering

Keep merging closest pairs



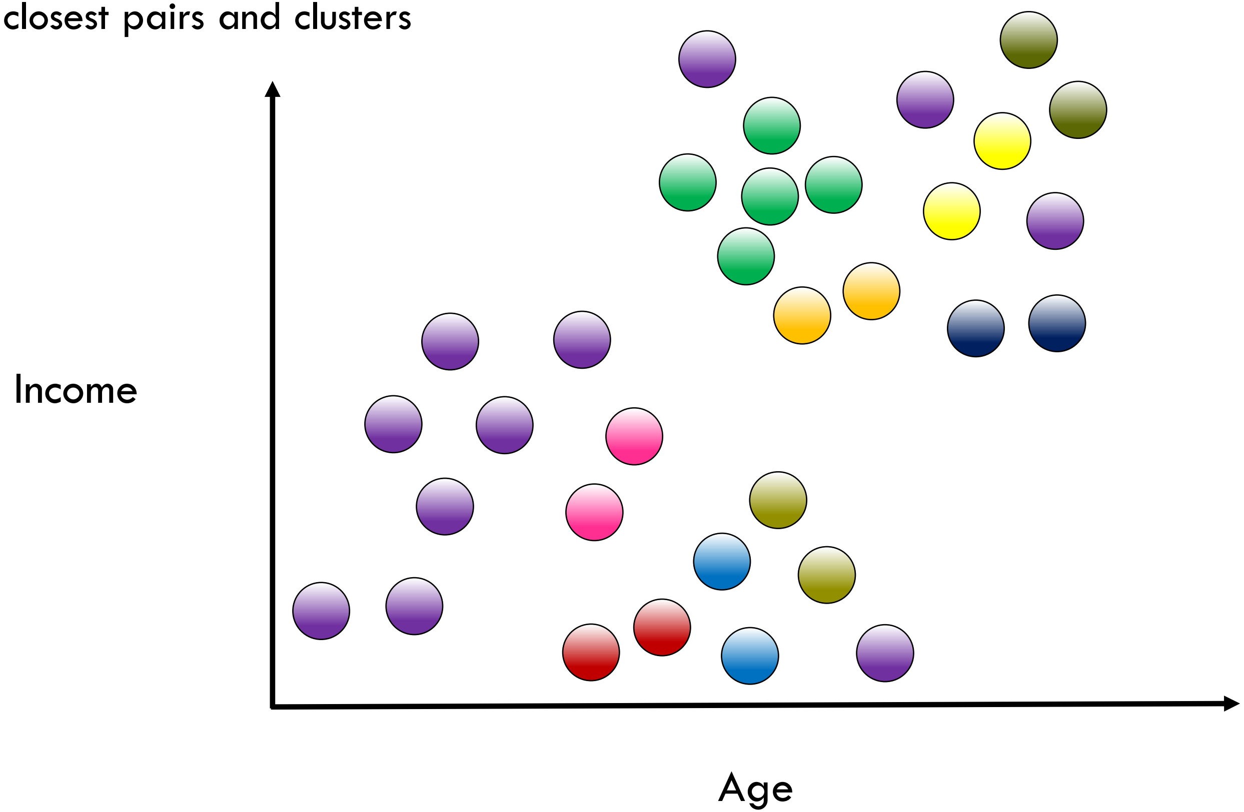
Hierarchical Agglomerative Clustering

If the closest pair is two clusters, merge them



Hierarchical Agglomerative Clustering

Keep merging closest pairs and clusters



Hierarchical Agglomerative Clustering

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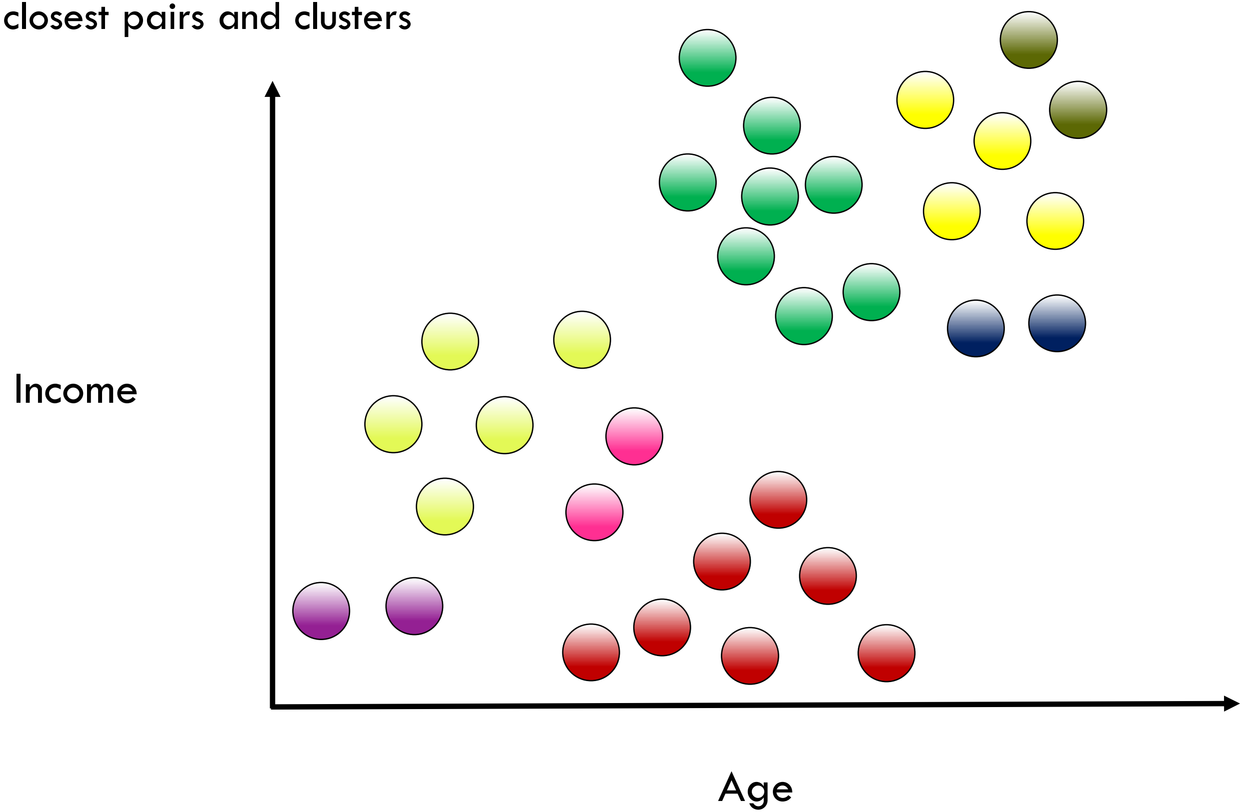
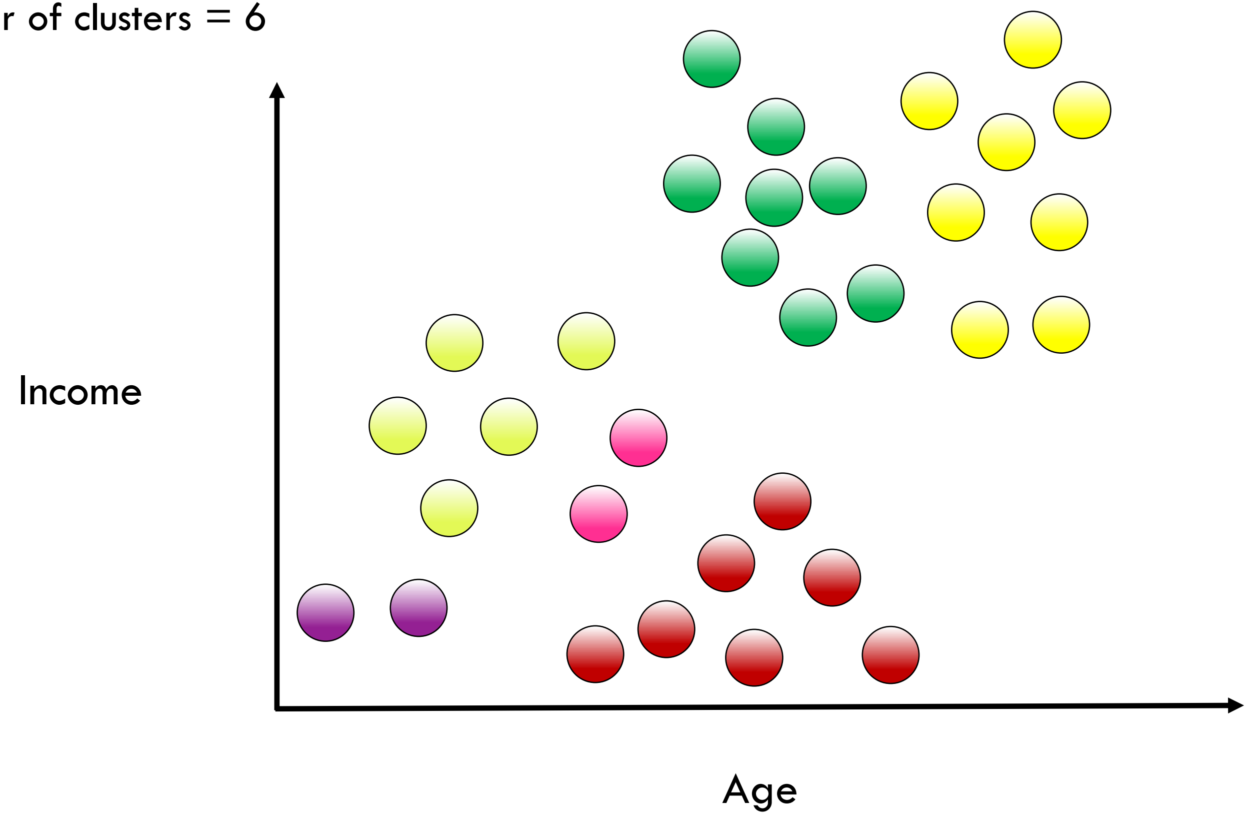


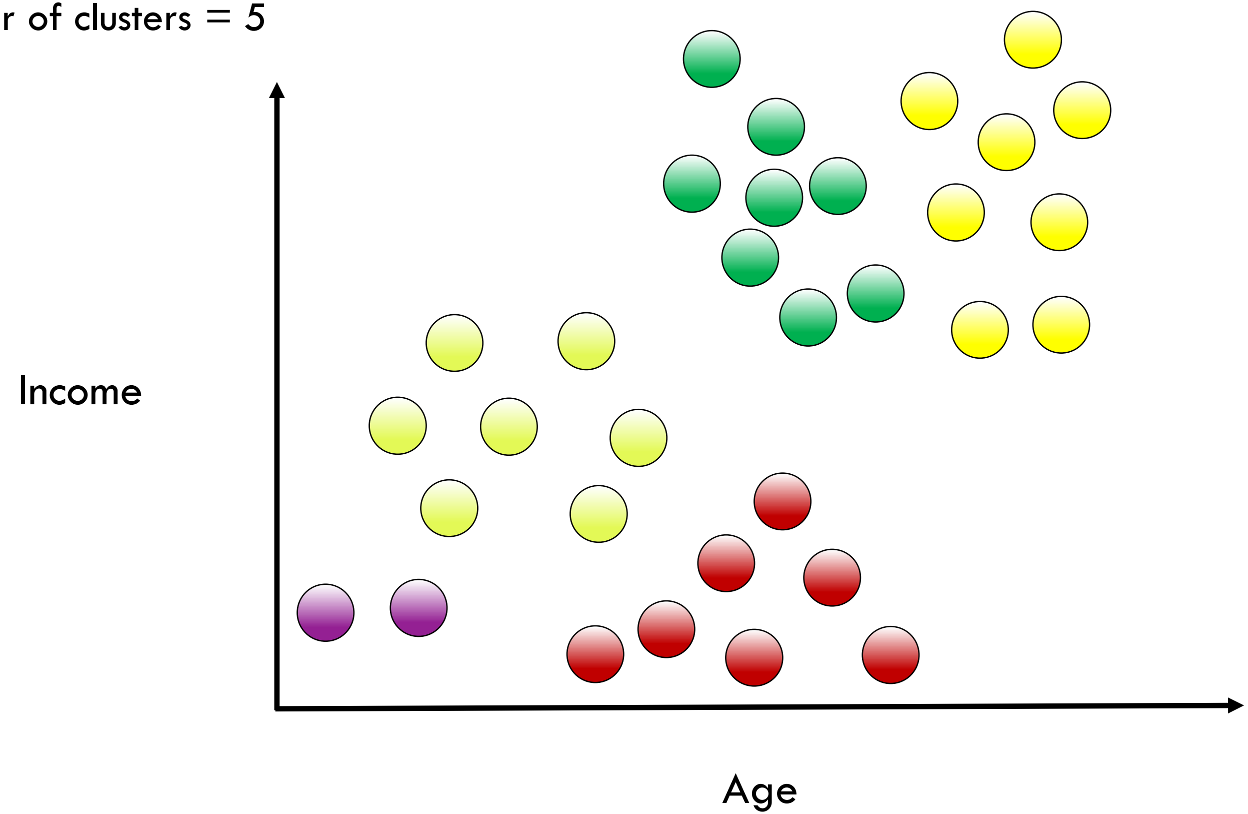
Hierarchical Agglomerative Clustering

Current number of clusters = 6



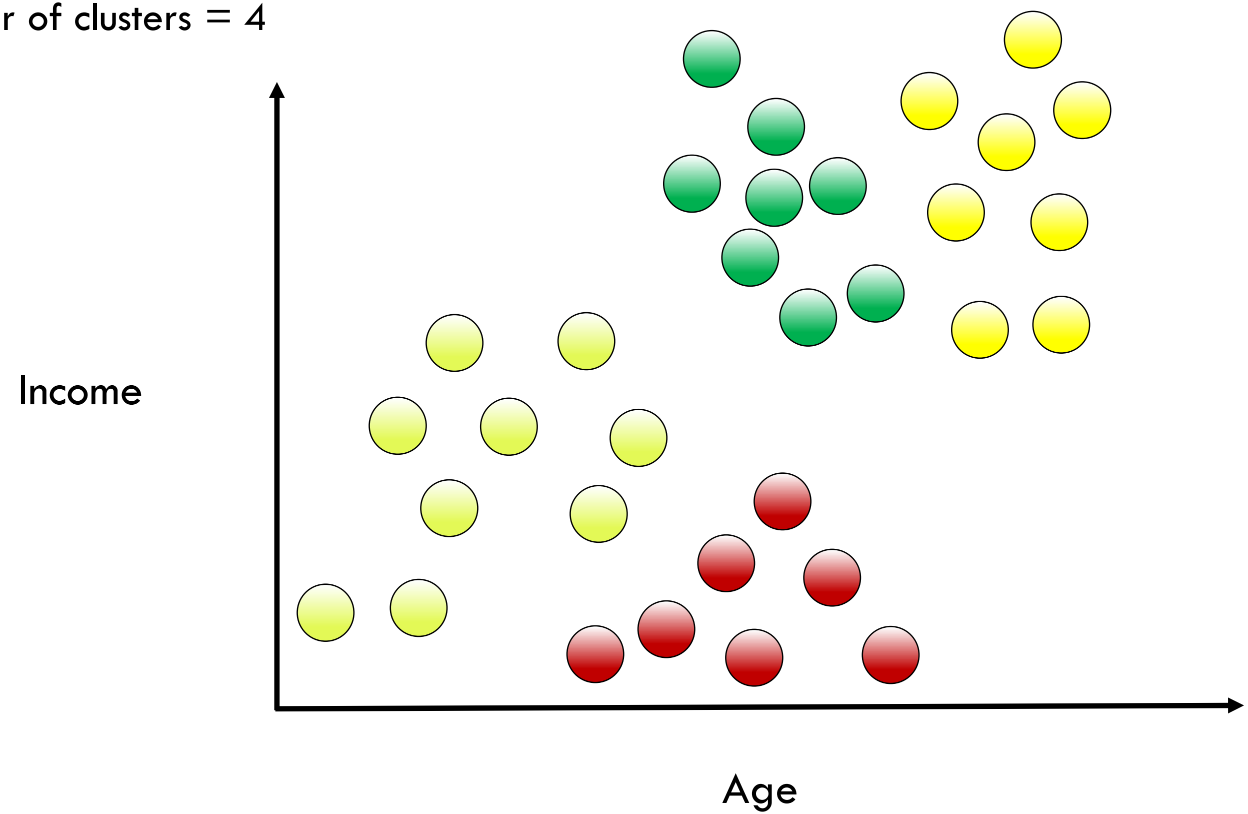
Hierarchical Agglomerative Clustering

Current number of clusters = 5



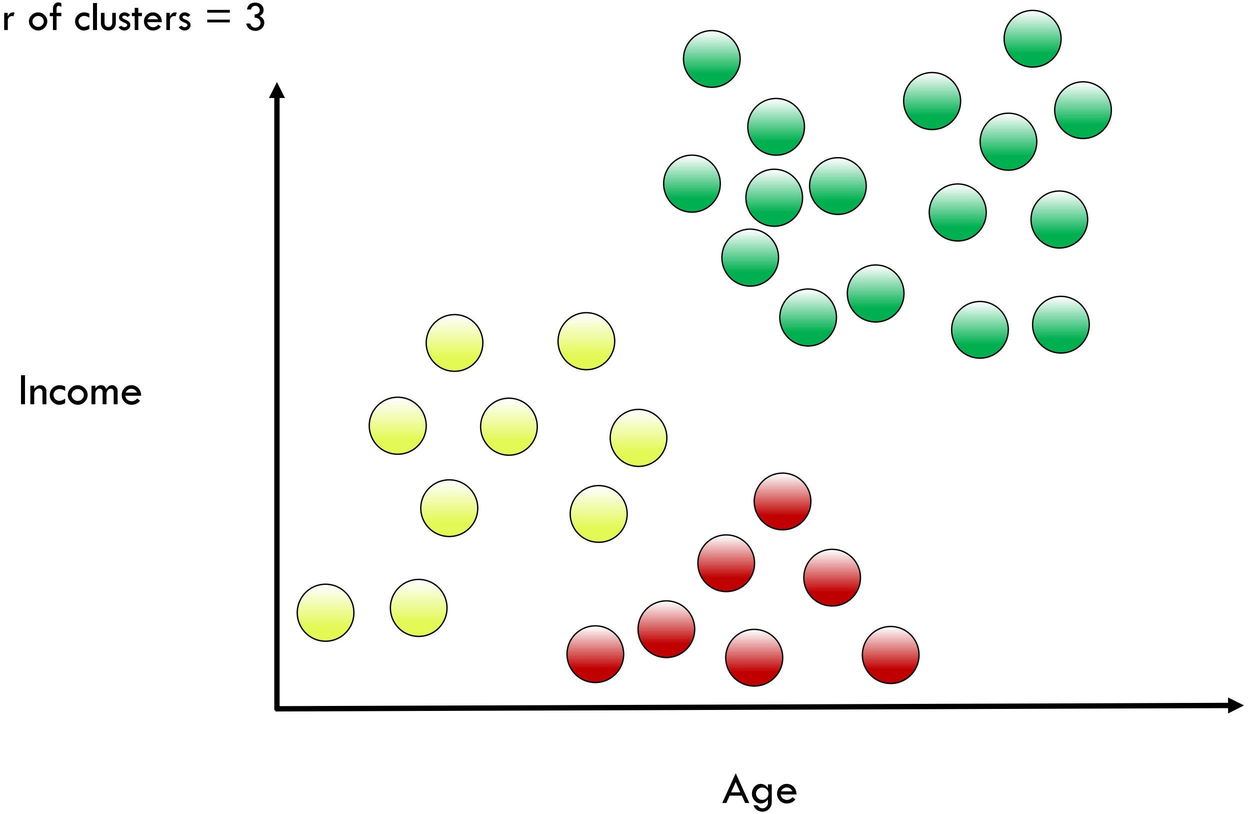
Hierarchical Agglomerative Clustering

Current number of clusters = 4



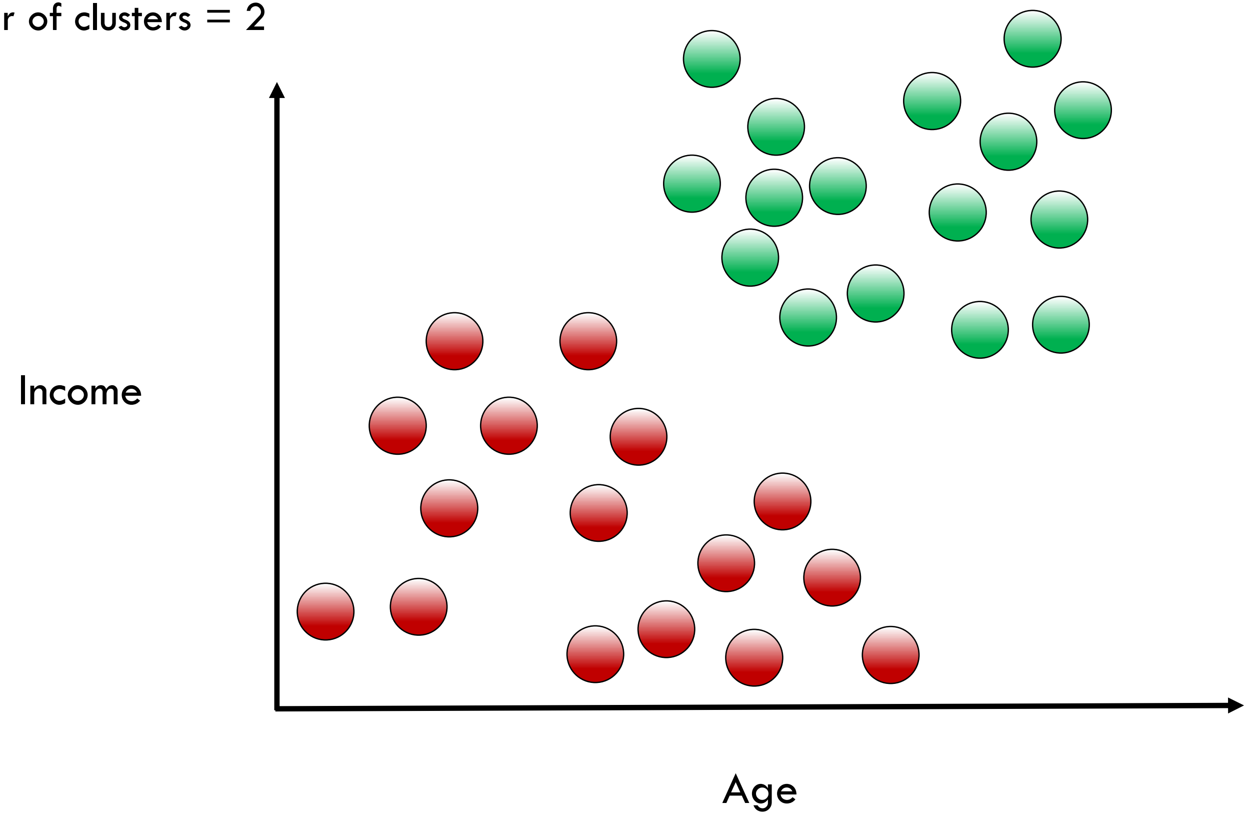
Hierarchical Agglomerative Clustering

Current number of clusters = 3



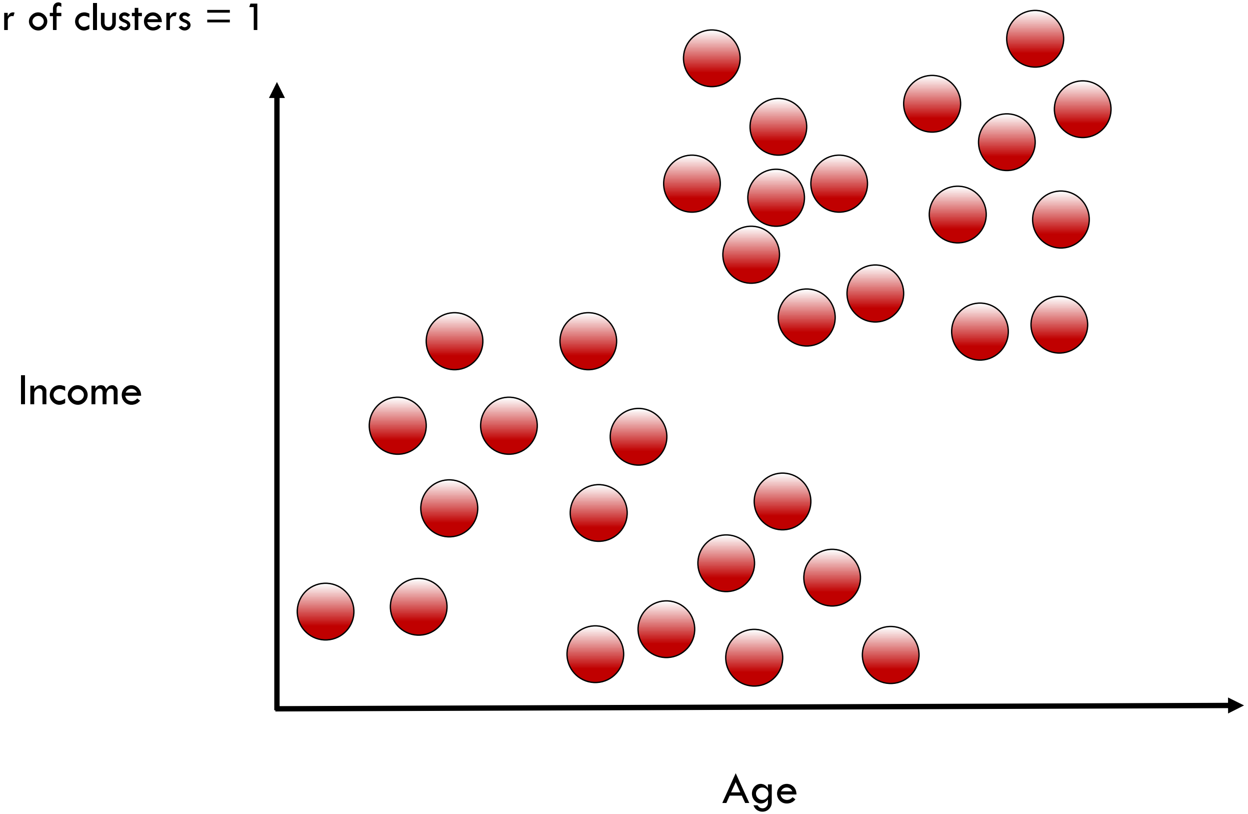
Hierarchical Agglomerative Clustering

Current number of clusters = 2



Hierarchical Agglomerative Clustering

Current number of clusters = 1



Agglomerative Clustering Stopping Conditions

Condition 1

the correct number of clusters is reached

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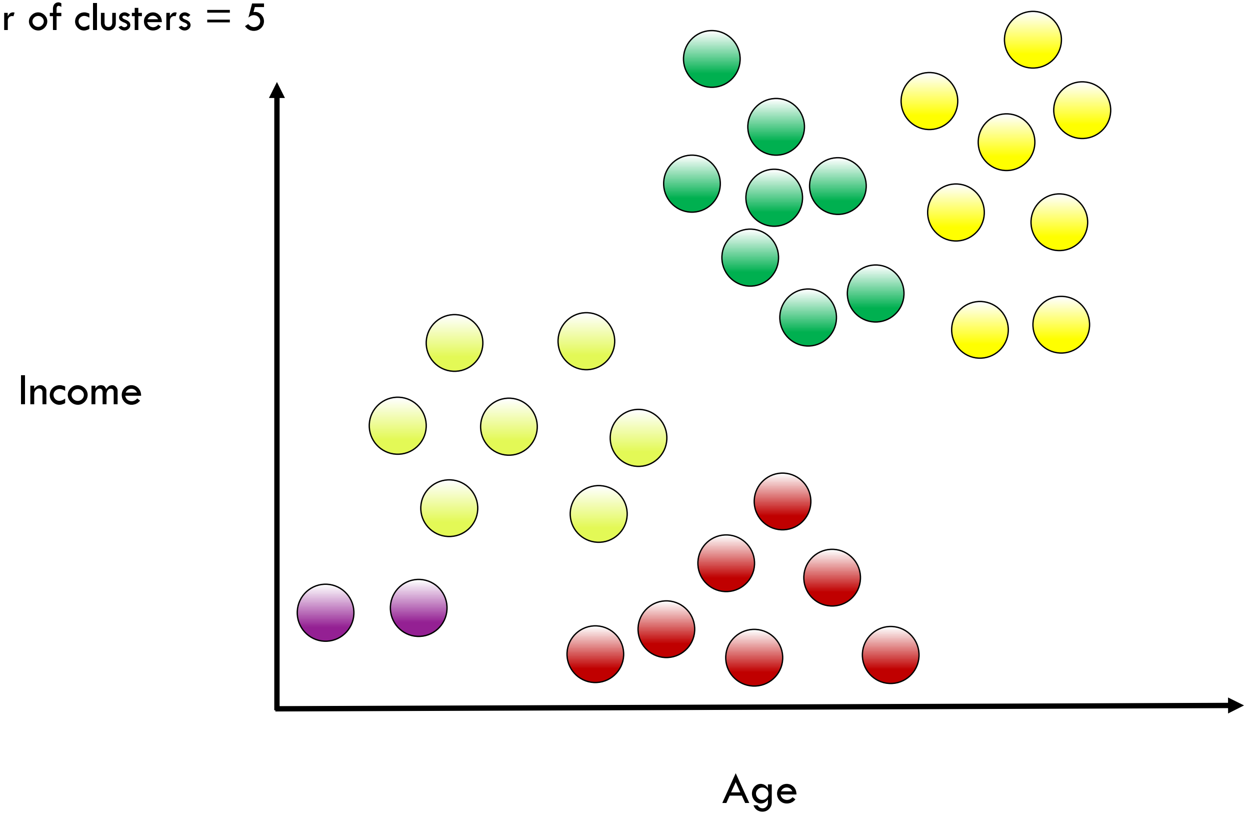
the correct number of clusters is reached

Condition 2

minimum average cluster distance reaches a set value

Hierarchical Agglomerative Clustering

Current number of clusters = 5

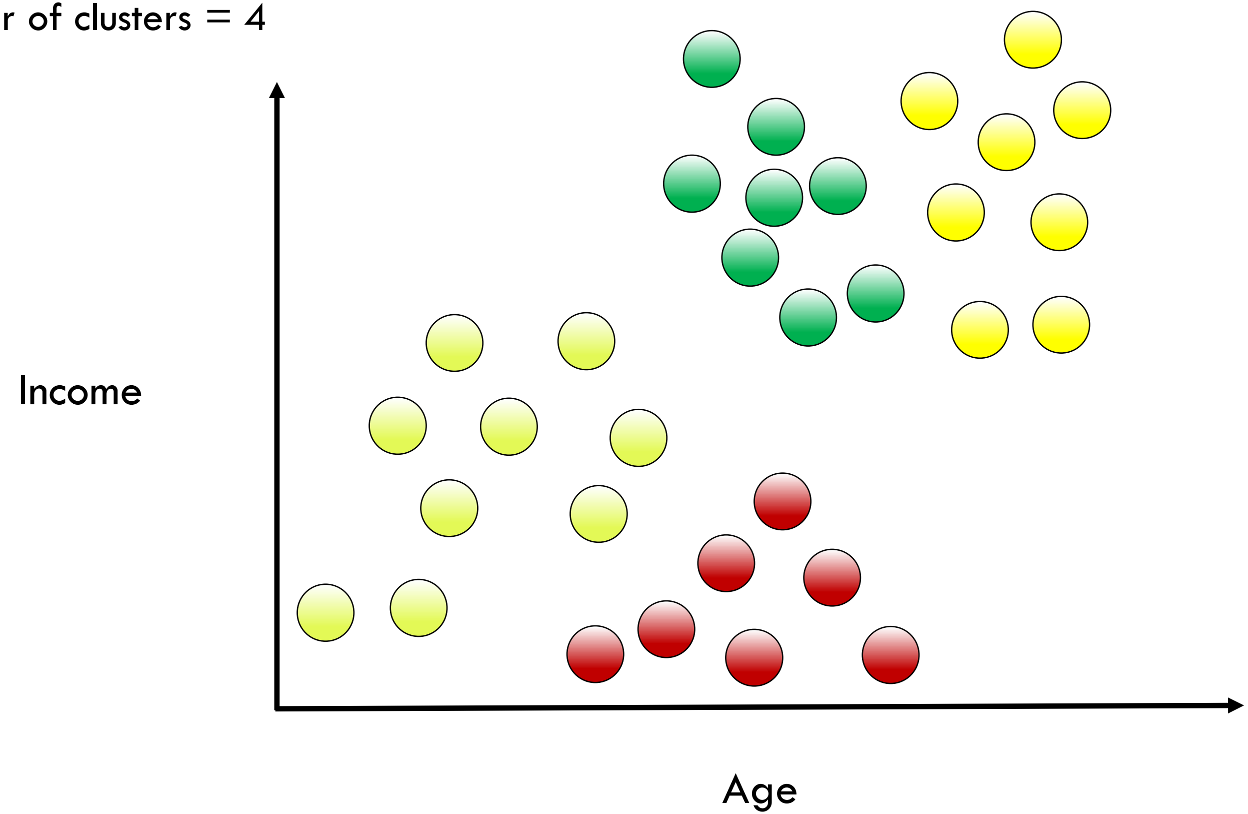


Hierarchical Agglomerative Clustering

Current number of clusters = 5

Hierarchical Agglomerative Clustering

Current number of clusters = 4

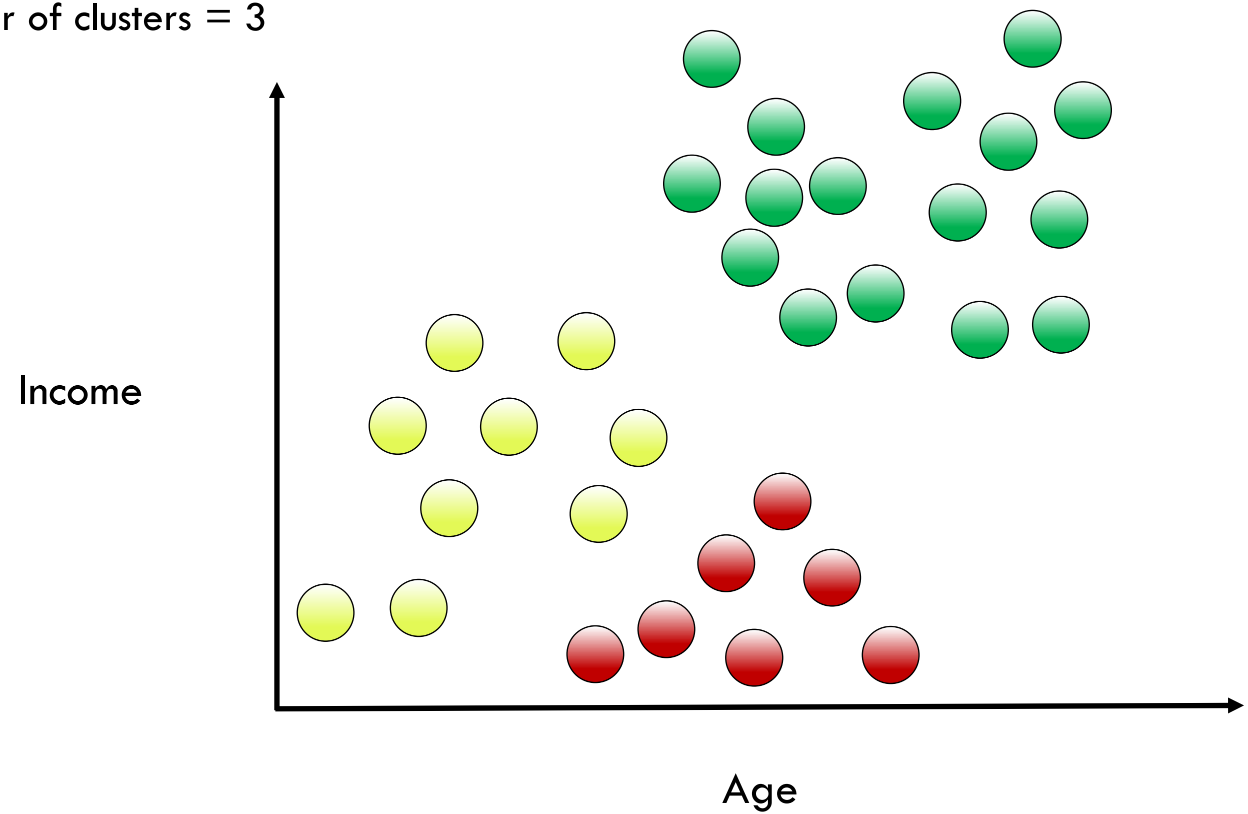


Hierarchical Agglomerative Clustering

Current number of clusters = 4

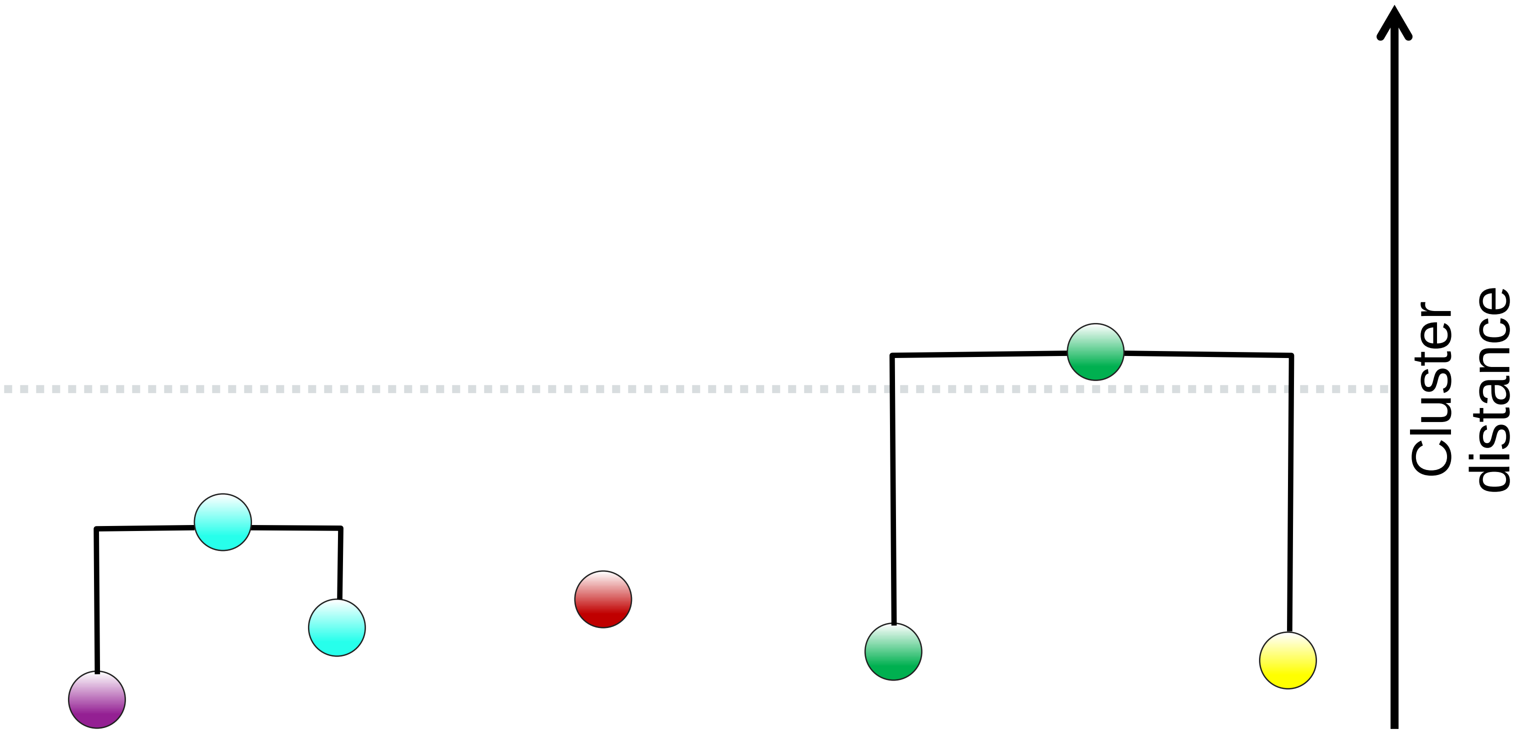
Hierarchical Agglomerative Clustering

Current number of clusters = 3



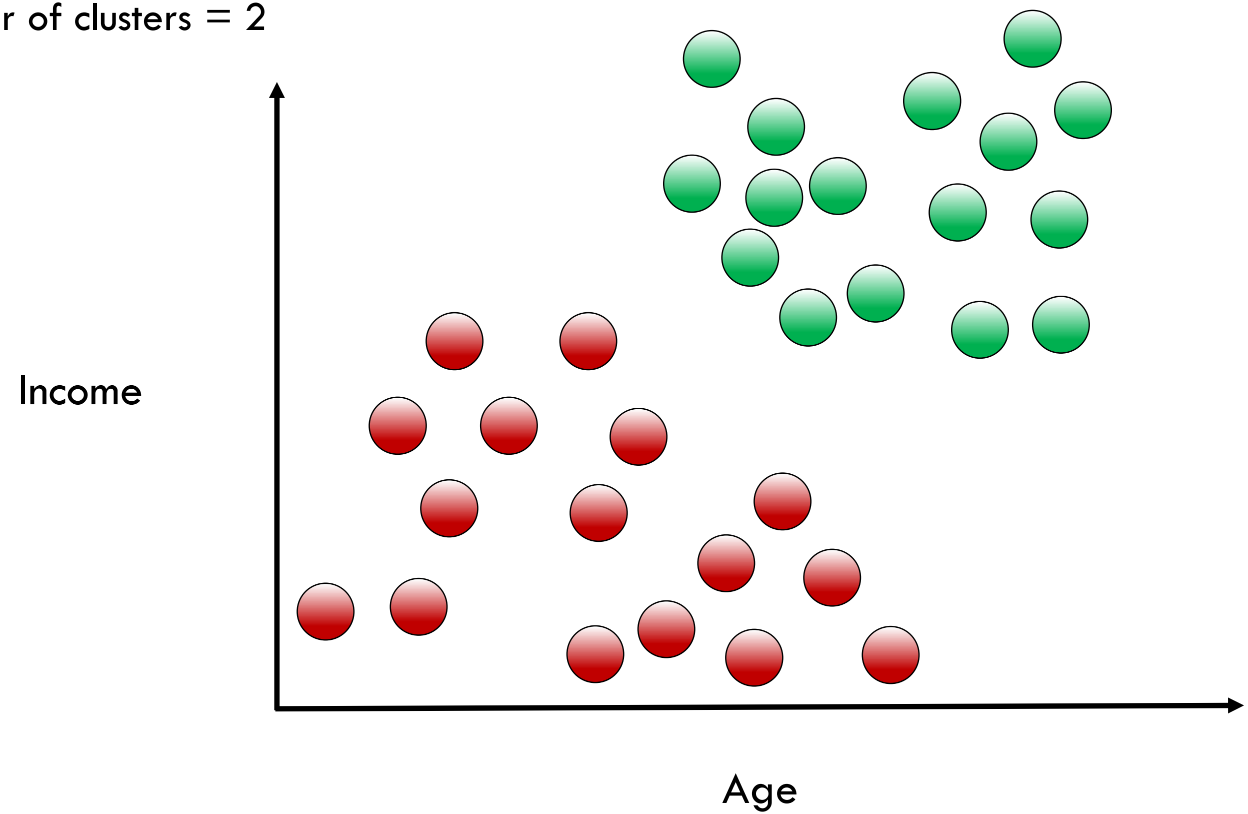
Hierarchical Agglomerative Clustering

Current number of clusters = 3



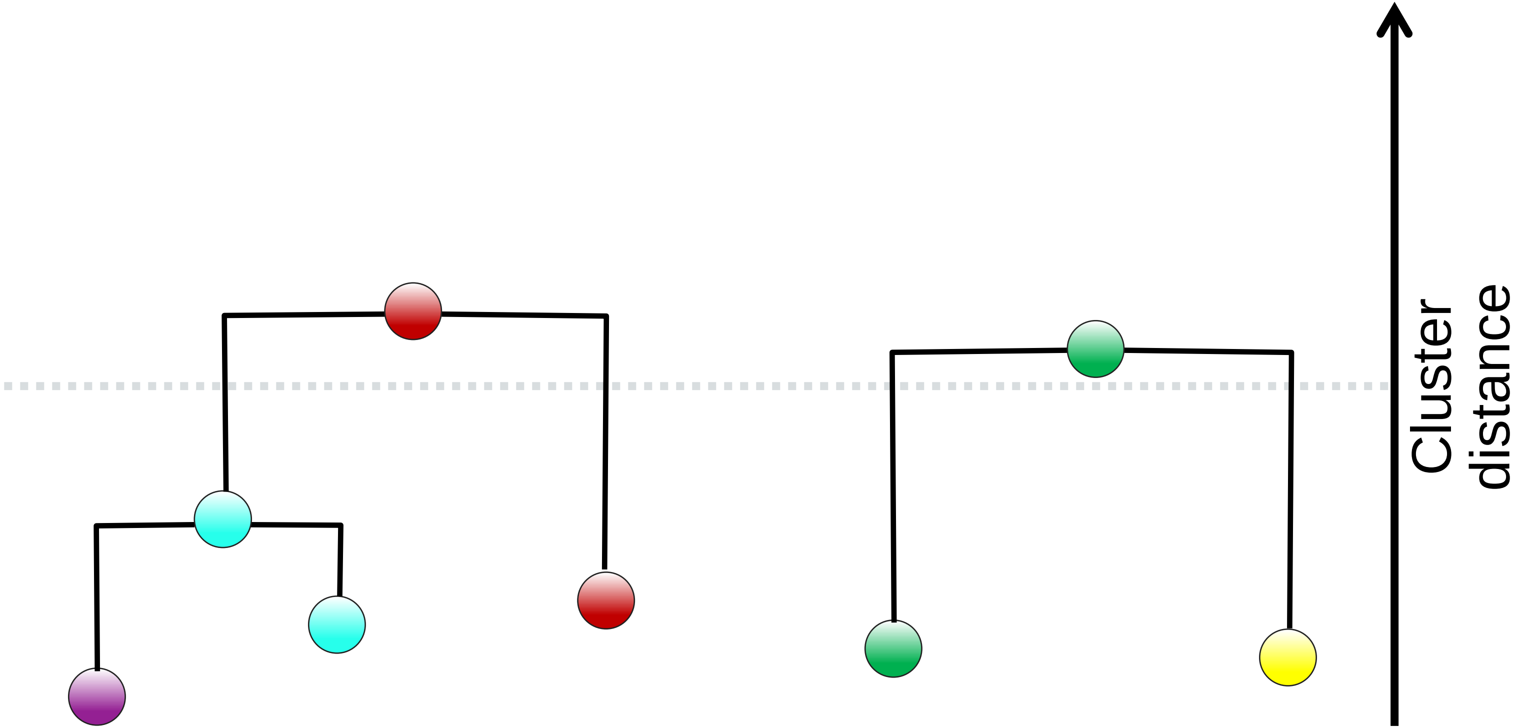
Hierarchical Agglomerative Clustering

Current number of clusters = 2



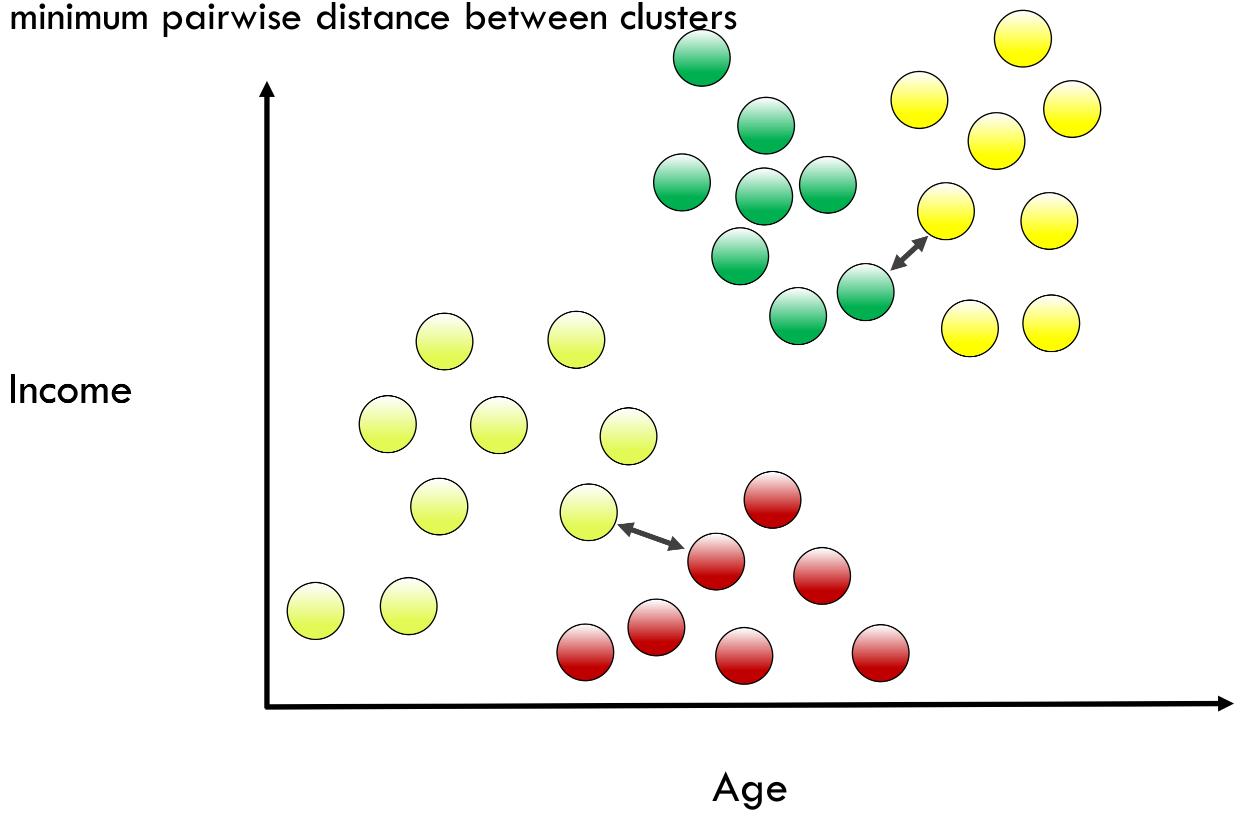
Hierarchical Agglomerative Clustering

Current number of clusters = 2



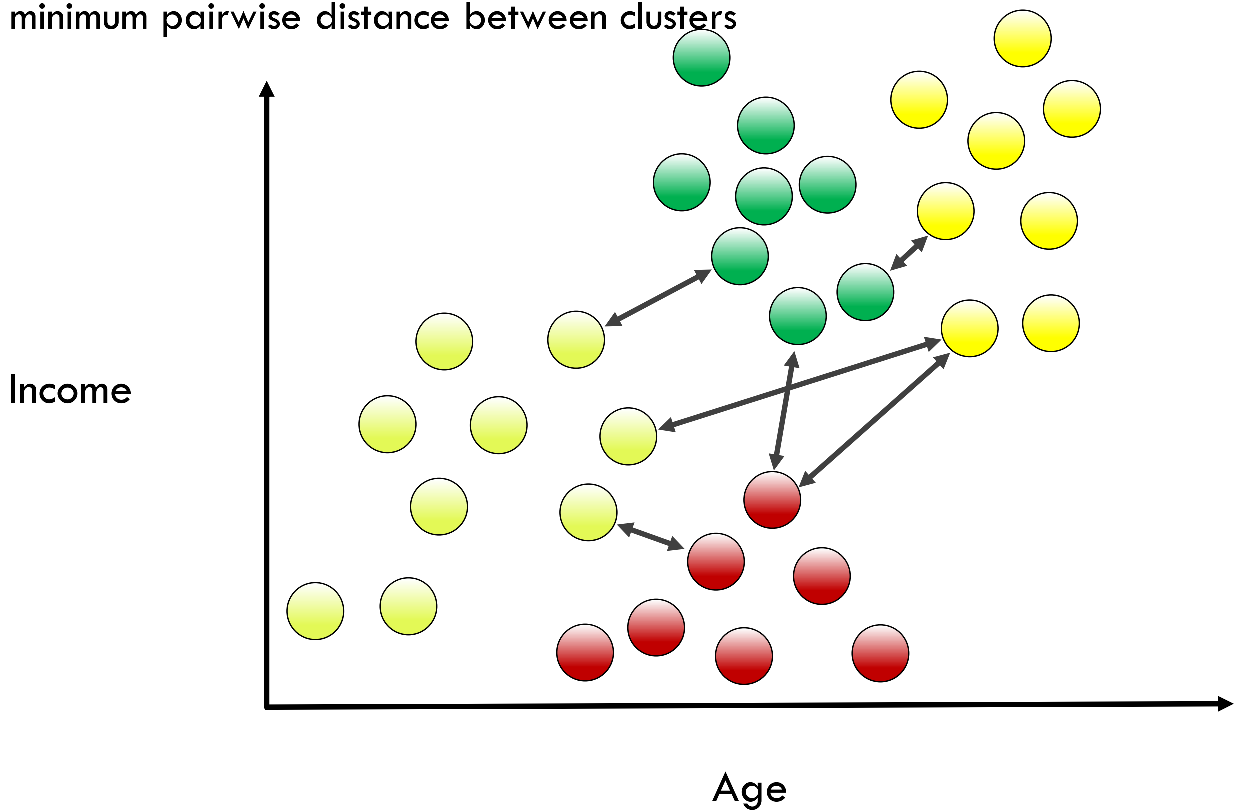
Hierarchical Linkage Types

<u>Single</u> linkage: minimum pairwise distance between clusters



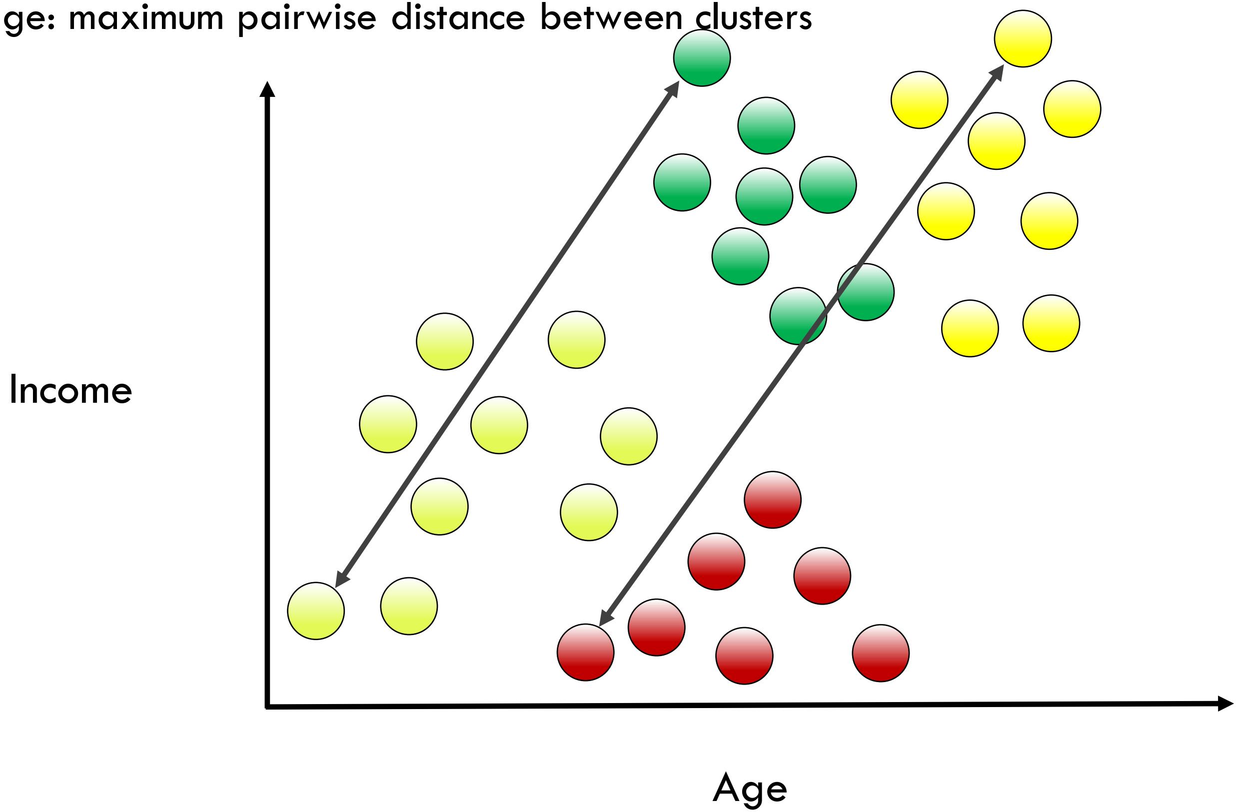
Hierarchical Linkage Types

<u>Single</u> linkage: minimum pairwise distance between clusters



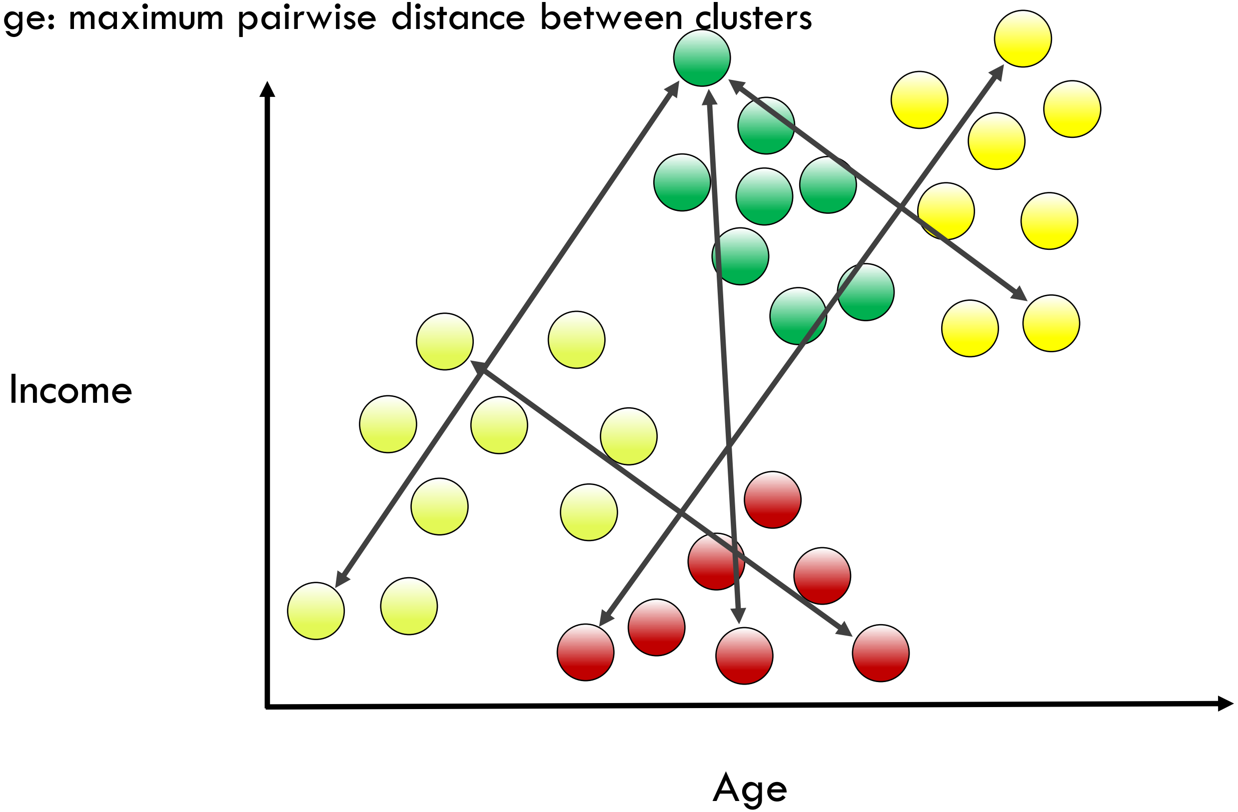
Hierarchical Linkage Types

Complete linkage: maximum pairwise distance between clusters



Hierarchical Linkage Types

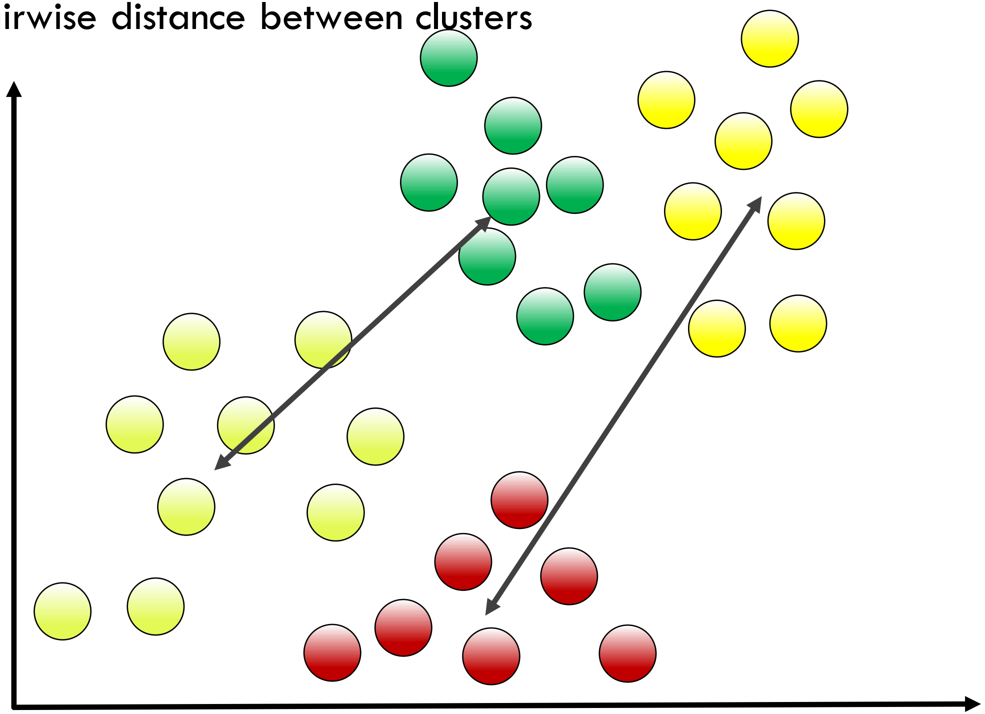
Complete linkage: maximum pairwise distance between clusters



Hierarchical Linkage Types

Average linkage: average pairwise distance between clusters

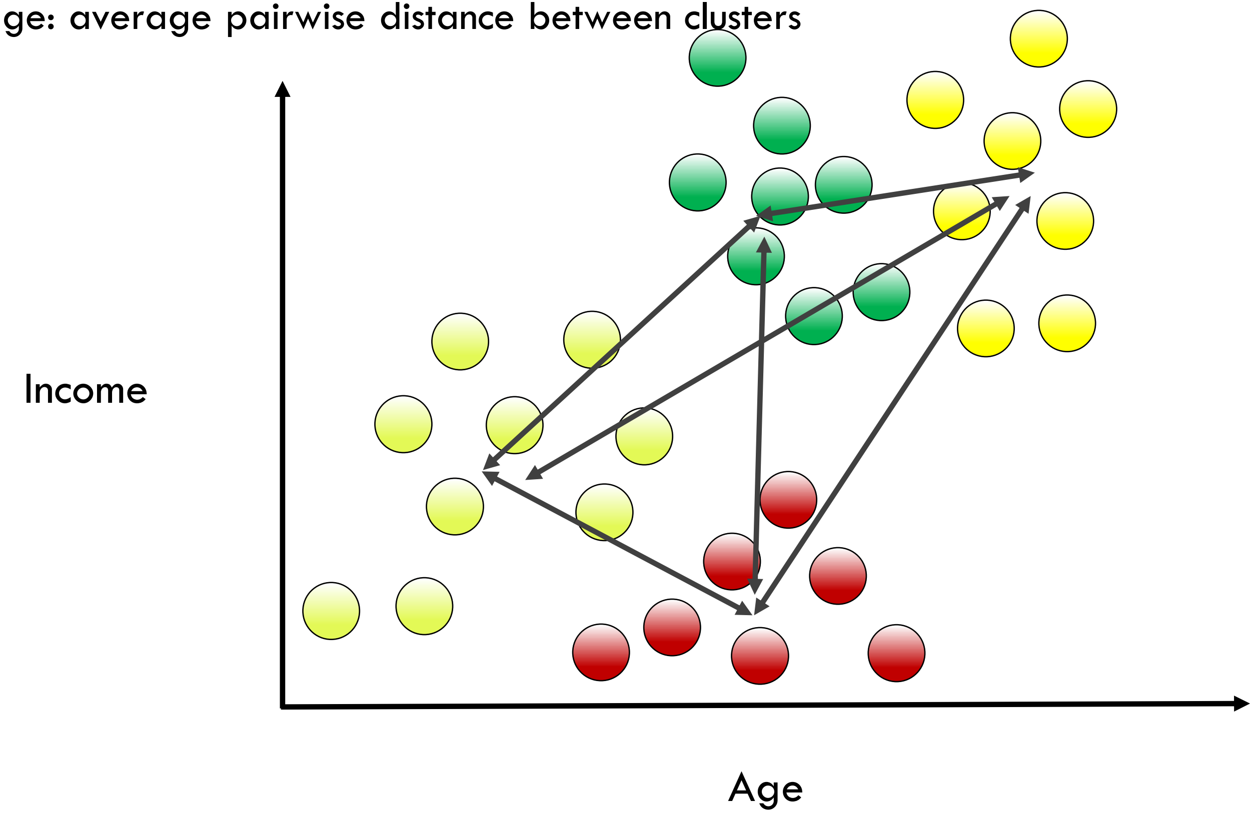
Income



Age

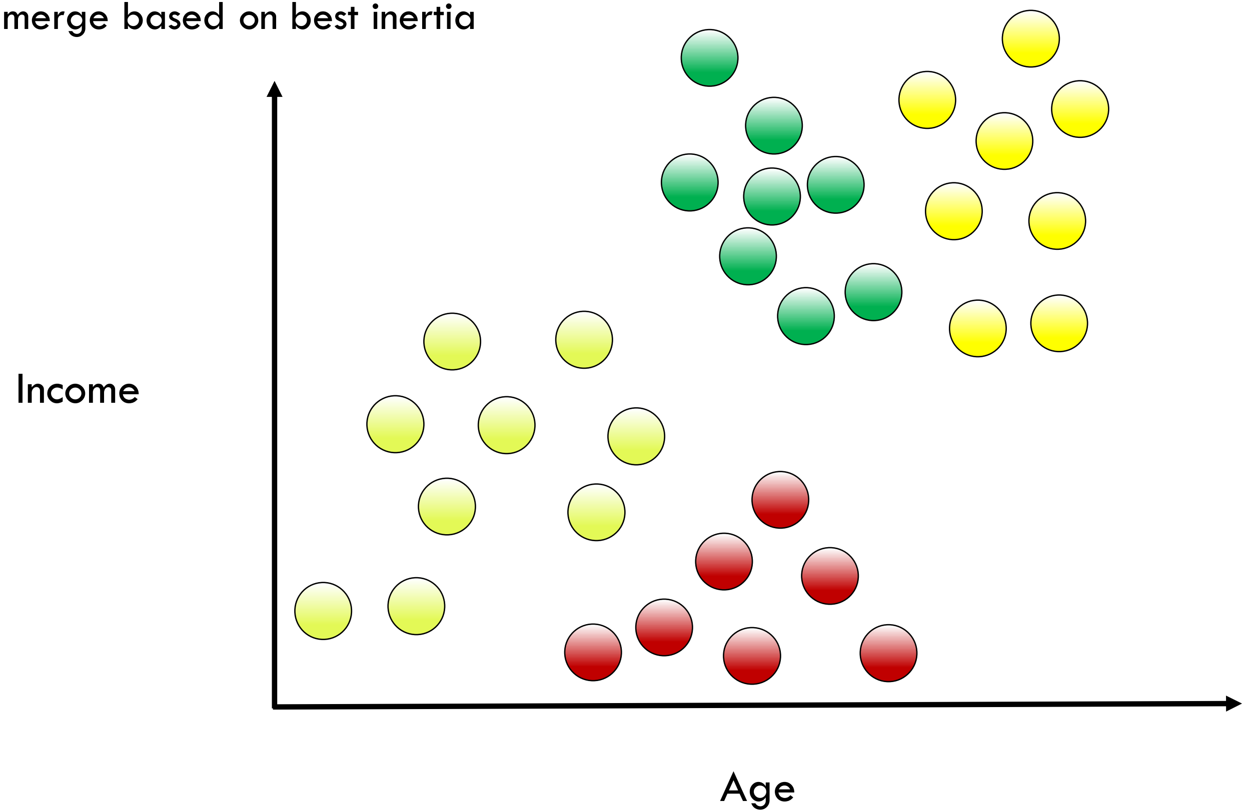
Hierarchical Linkage Types

<u>Average</u> linkage: average pairwise distance between clusters



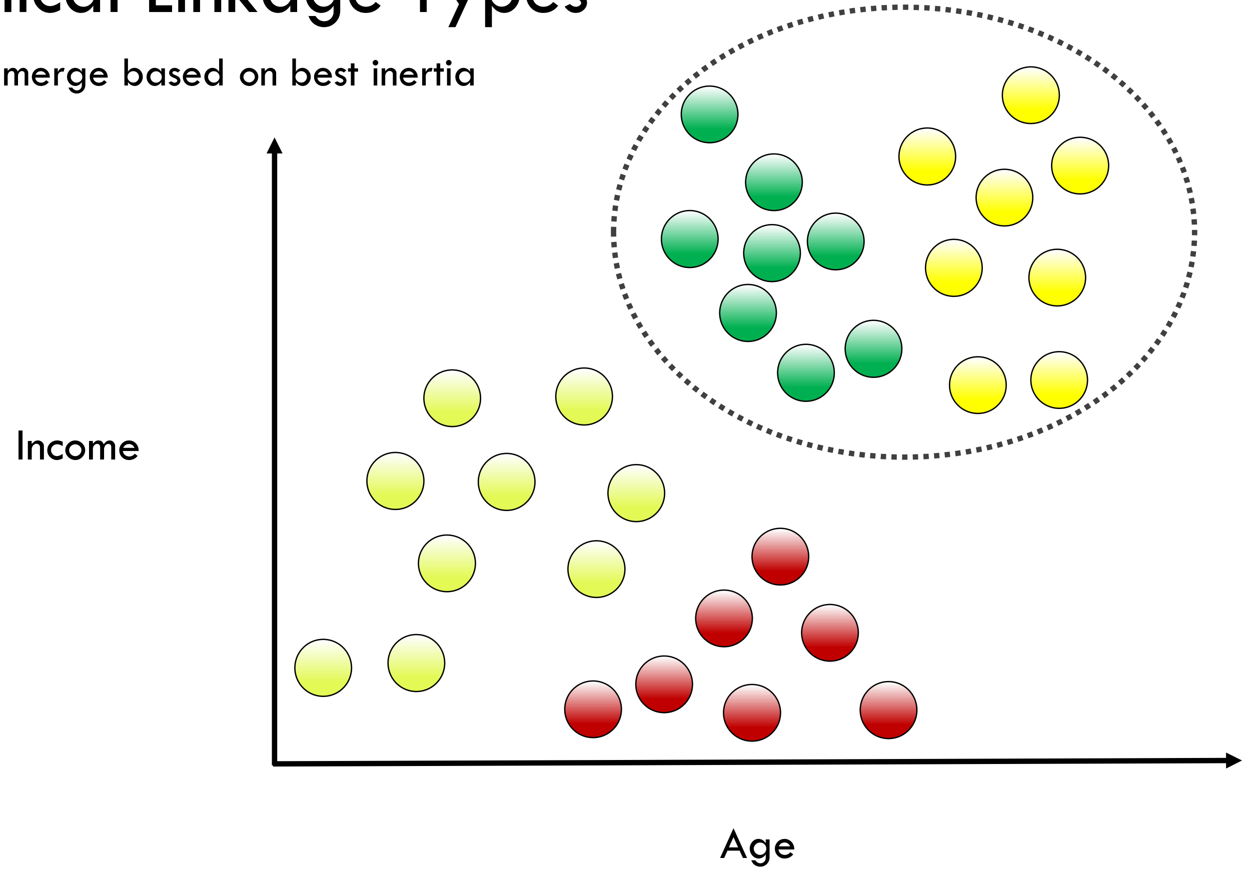
Hierarchical Linkage Types

Ward linkage: merge based on best inertia



Hierarchical Linkage Types

Ward linkage: merge based on best inertia



Agglomerative Clustering: The Syntax

Import the class containing the clustering method

```
from sklearn.cluster import AgglomerativeClustering
```

Create an instance of the class

```
agg = AgglomerativeClustering(n_clusters=3,
                              affinity='euclidean',
                              linkage='ward')
```

Fit the instance on the data and then predict clusters for new data

```
agg = agg.fit(X1)
y_predict = agg.predict(X2)
```

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final number of clusters

Fit the instance on the data and then predict clusters for new data

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Agglomerative Clustering: The Syntax

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Create an instance of the class

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                              linkage='ward')
```

cluster affinity and aggregation

Fit the instance on the data and then predict clusters for new data

```
agg = agg.fit(X1)
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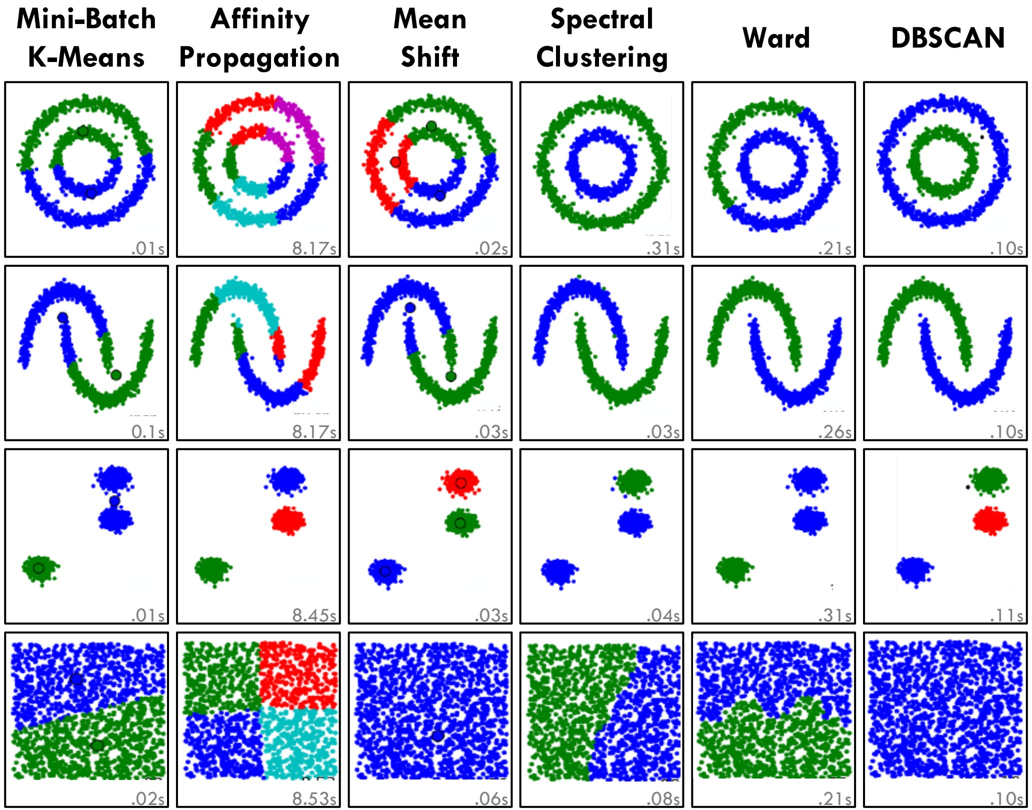
```

Other Types of Clustering



Reference: http://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html

Software